LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022217\
Data File : BF093094.D
Acq On : 22 Feb 2017 23:55
Operator : SJ/MA
Sample : I1931-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-6

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	3.093	85	88	103	rBV	85155	235807	1.01%	0.361%
2	3.344	107	110	122	rVB	425154	845768	3.64%	1.294%
3	3.756	142	146	156	rVB	350251	575352	2.48%	0.881%
4	4.396	194	202	205	rBV	6295568	23241016	100.00%	35.569%
5	5.059	253	260	262	rBV	4704371	13139047	56.53%	20.109%
6	6.476	382	384	390	rBV	297159	335841	1.45%	0.514%
7	6.842	413	416	418	rBV	1015819	1006265	4.33%	1.540%
8	7.002	427	430	432	rBV	2745067	3331453	14.33%	5.099%
9	7.162	442	444	447	rBV	428001	619159	2.66%	0.948%
10	7.413	463	466	468	rBV	2699033	2939291	12.65%	4.498%
11	8.122	526	528	531	rBV	1314909	1365608	5.88%	2.090%
12	9.196	619	622	625	rBV	3482488	4767874	20.51%	7.297%
13	9.596	655	657	659	rBV	704683	671976	2.89%	1.028%
14	9.870	679	681	683	rVV	1617754	1526839	6.57%	2.337%
15	10.773	758	760	764	rBV2	229337	304718	1.31%	0.466%
16	11.356	808	811	812	rBV	1615232	1601413	6.89%	2.451%
17	11.585	828	831	835	rBV2	123960	235109	1.01%	0.360%
18	11.916	858	860	862	rBV	310429	256311	1.10%	0.392%
19	12.568	914	917	919	rBV	438347	536132	2.31%	0.821%
20	12.785	933	936	939	rBV2	300409	493183	2.12%	0.755%
21	12.945	947	950	952	rVB	3363364	4376285	18.83%	6.698%
22	13.825	1025	1027	1033	rVB	185658	272322	1.17%	0.417%
23	13.985	1038	1041	1048	rVB2	1345293	1622005	6.98%	2.482%
24	15.414	1163	1166	1172	rBV	731465	1041262	4.48%	1.594%

Sum of corrected areas: 65340036

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Misc :
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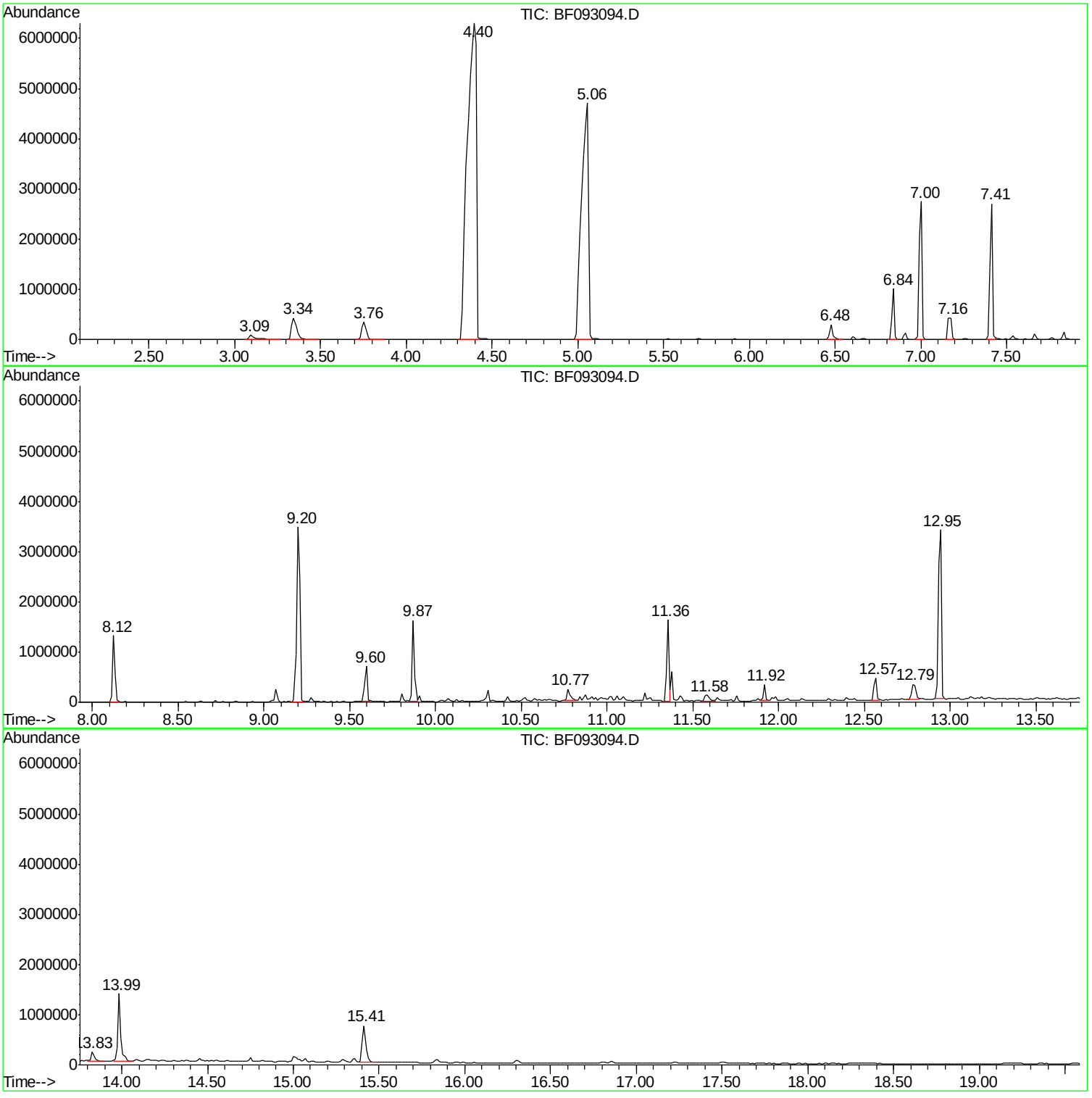
Instrument : BNA_F
ClientSampleId : P-6

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

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TIC Integration Parameters: LSCINT.P

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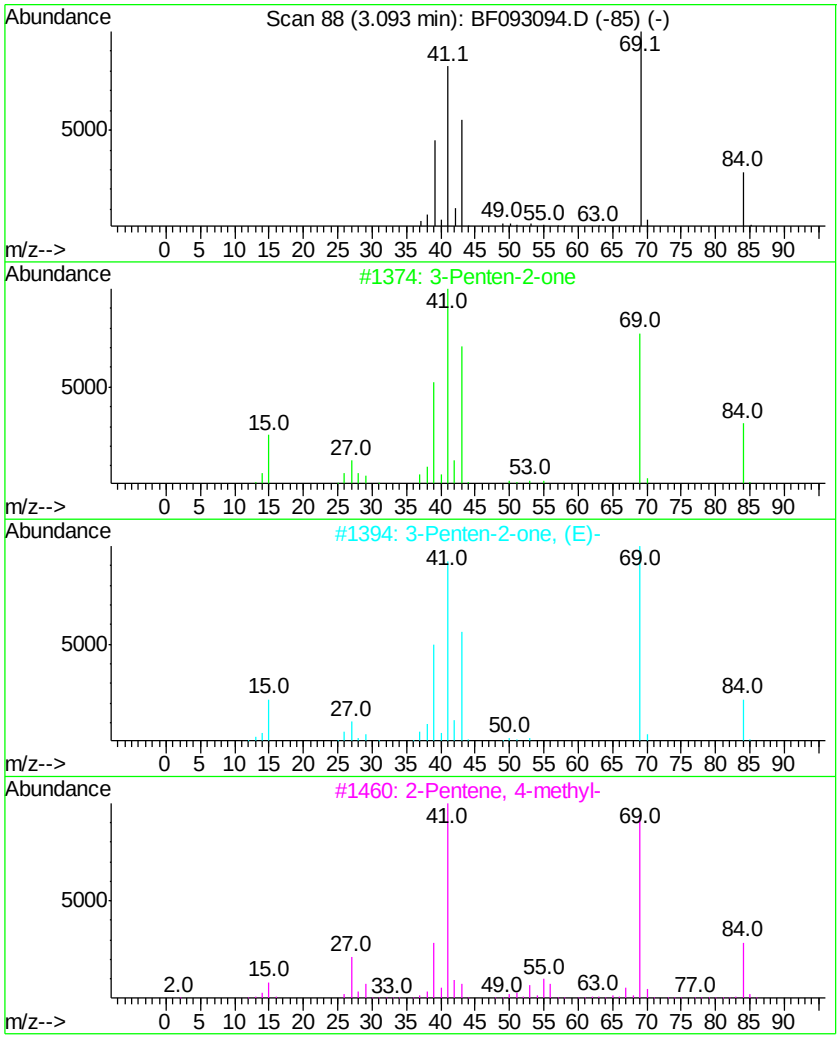
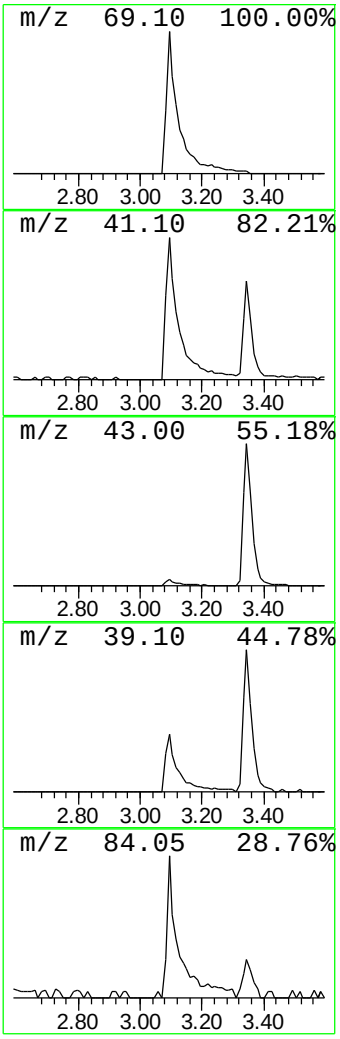
Peak Number 1 3-Penten-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.09	4.69 ng	235807	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one	84	C5H8O	000625-33-2	91
2	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	78
3	2-Pentene, 4-methyl-	84	C6H12	004461-48-7	58
4	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	58
5	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	58





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Operator : SJ/MA
Sample : I1931-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-6

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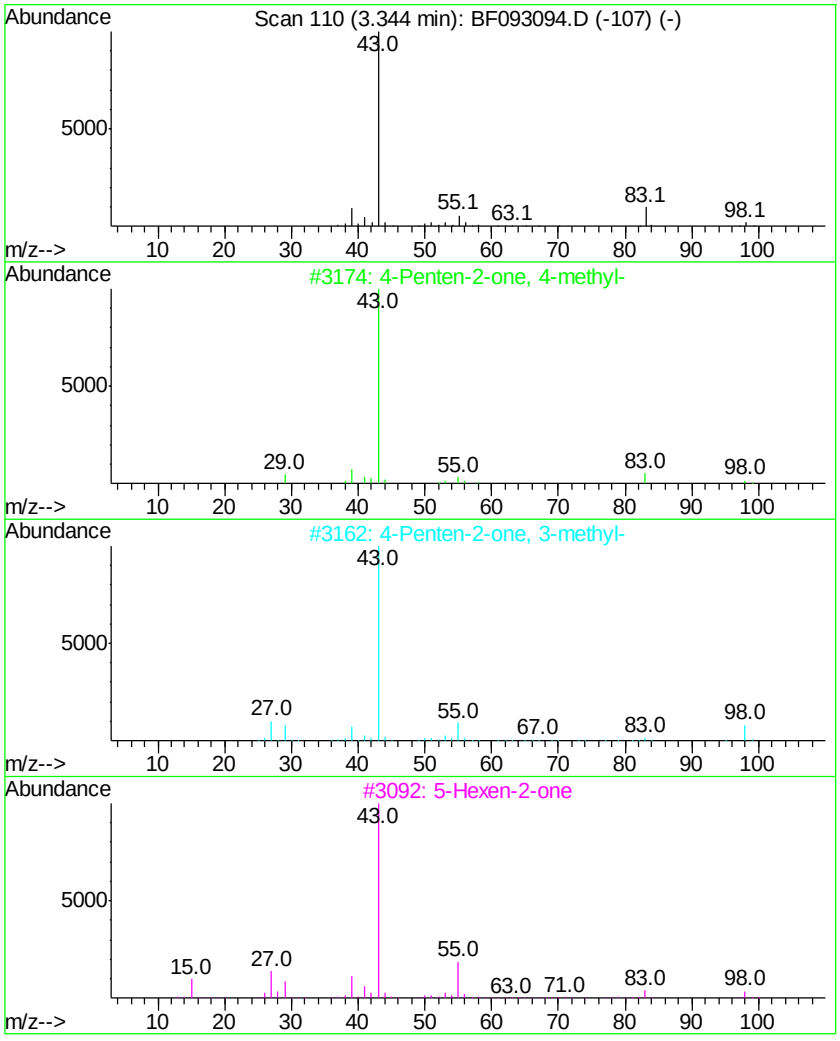
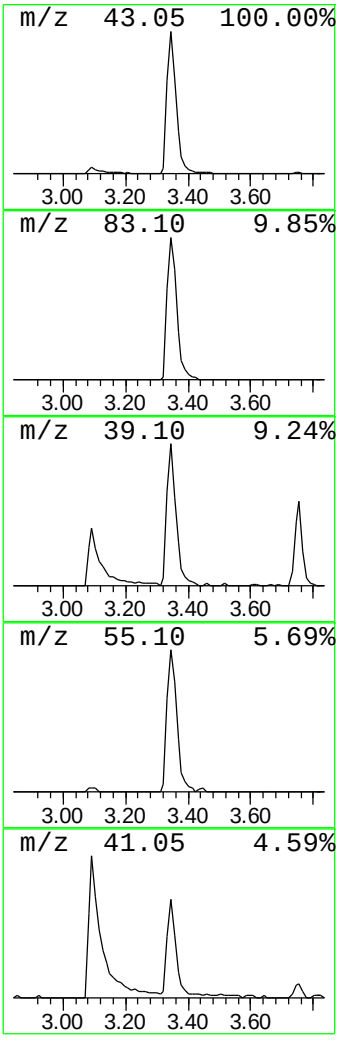
Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.34	16.81 ng	845768	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	47
3	5-Hexen-2-one	98	C6H10O	000109-49-9	35
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	28
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022217\
Data File : BF093094.D
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Operator : SJ/MA
Sample : I1931-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-6

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

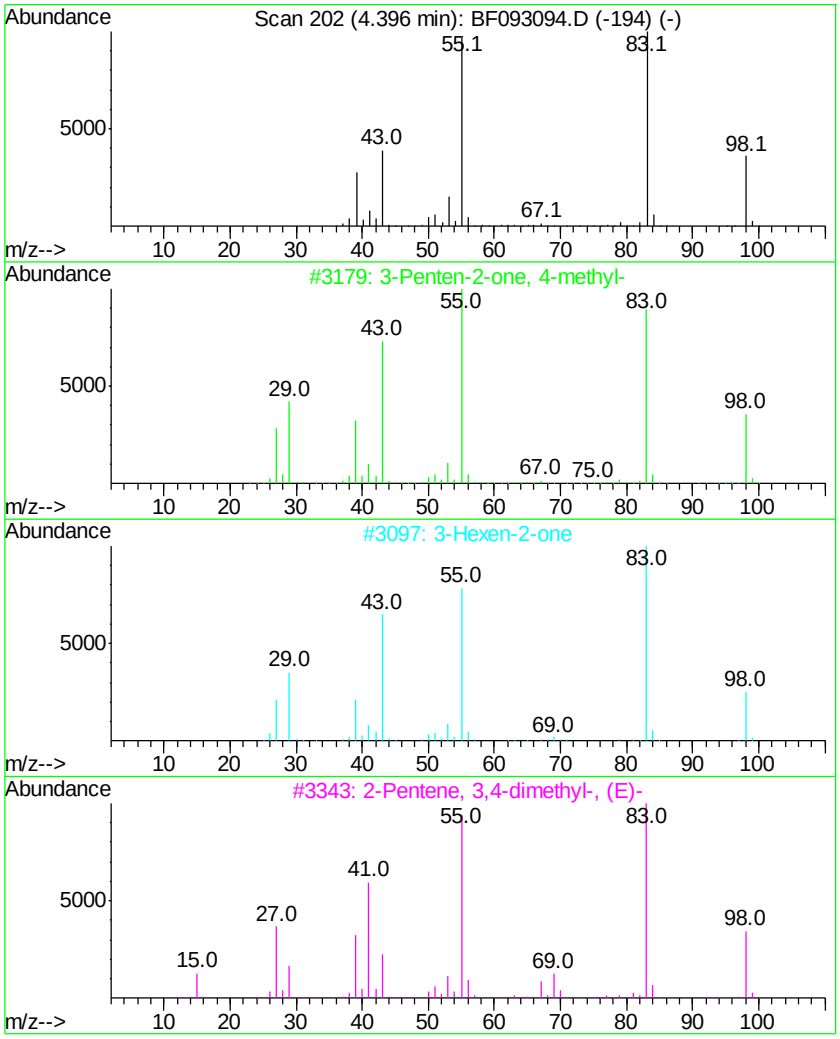
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

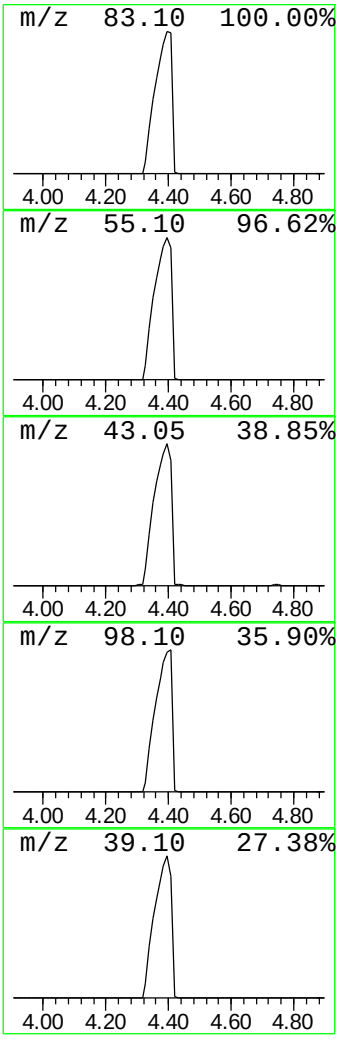
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	461.93 ng	23241000	1,4-Dichlorobenzene-d4	6.84

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, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





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Sample : I1931-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-6

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

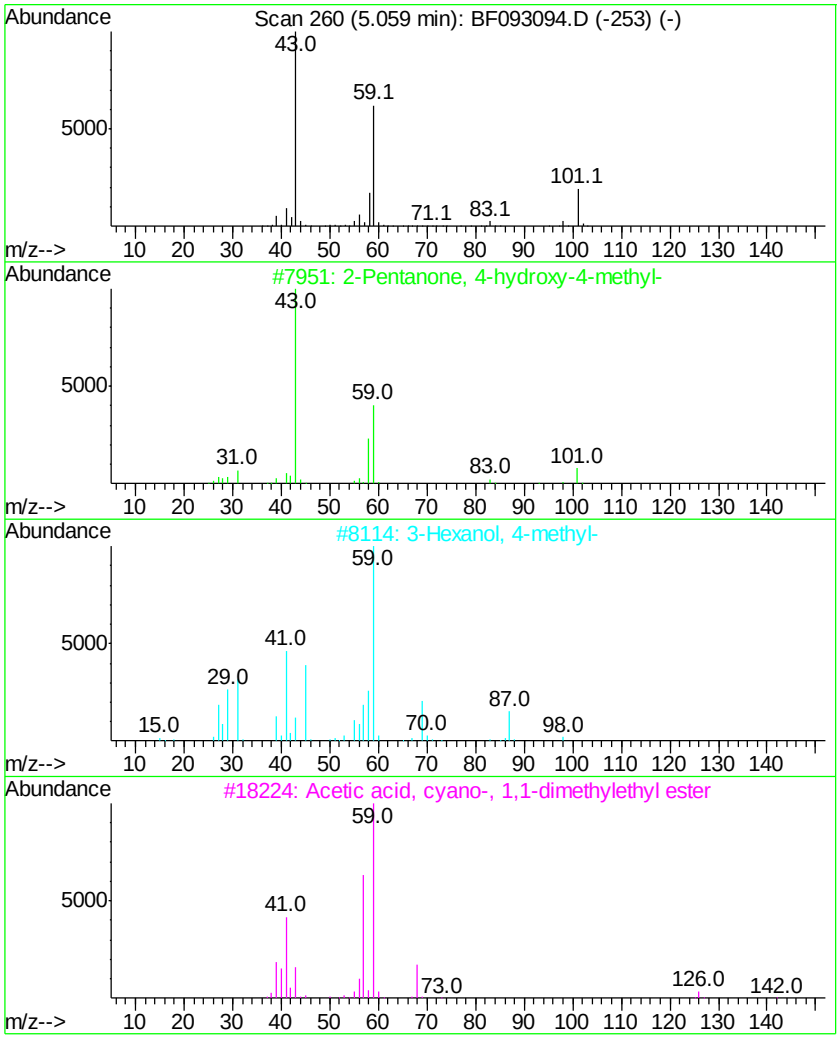
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

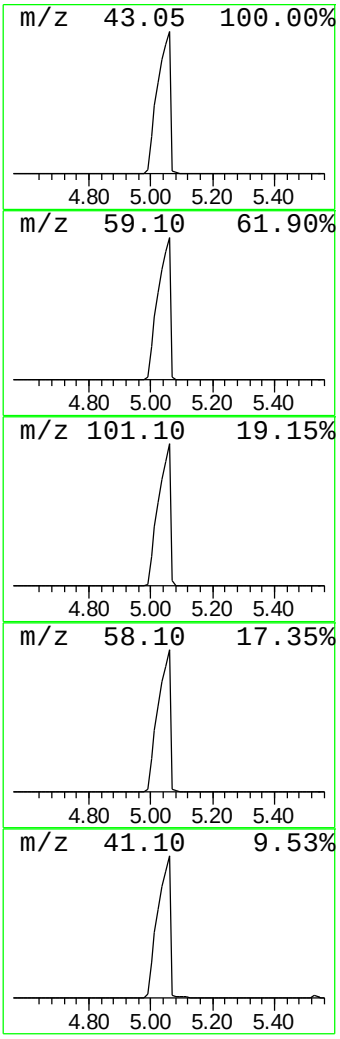
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	261.15 ng	13139000	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022217\
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Sample : I1931-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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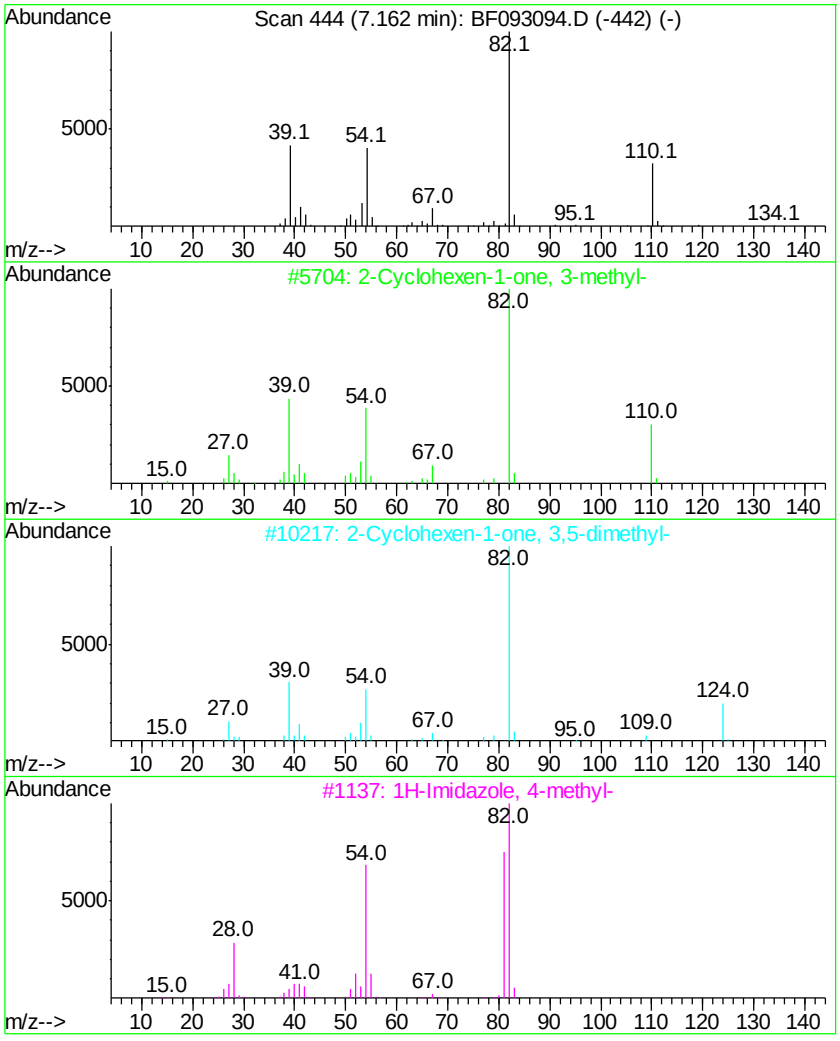
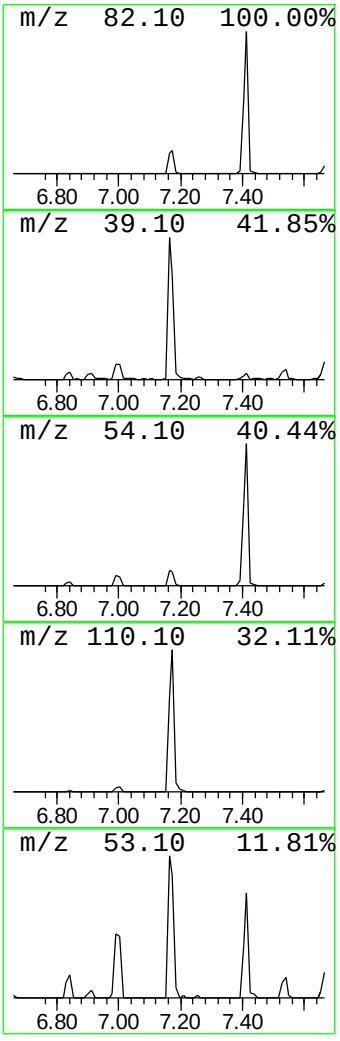
Peak Number 7 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	12.31 ng	619159	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	95
2	2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	53
3	1H-Imidazole, 4-methyl-	82	C4H6N2	000822-36-6	38
4	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	38
5	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	37





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TIC Library : C:\DATABASE\NIST02.L
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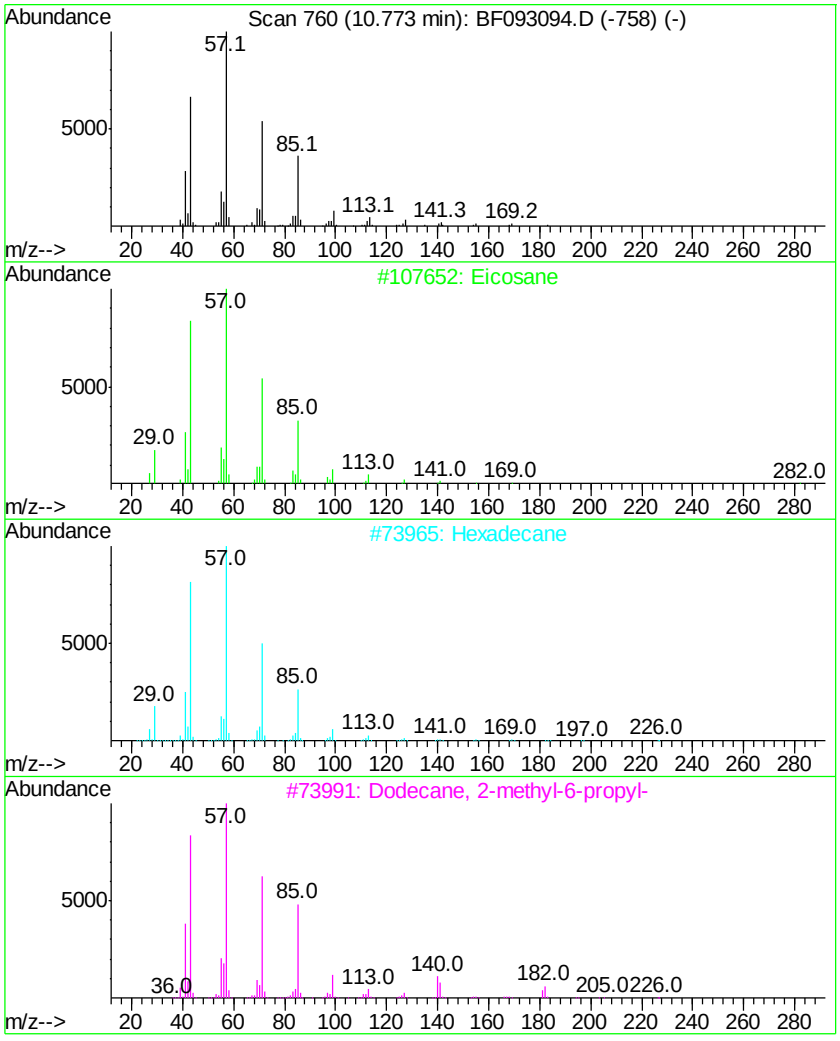
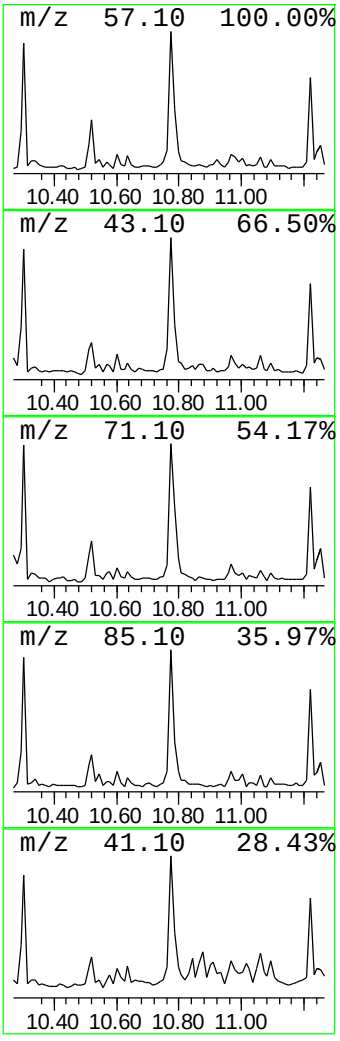
Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	3.81 ng	304718	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
4	Heptadecane	240	C17H36	000629-78-7	86
5	Pentadecane	212	C15H32	000629-62-9	86





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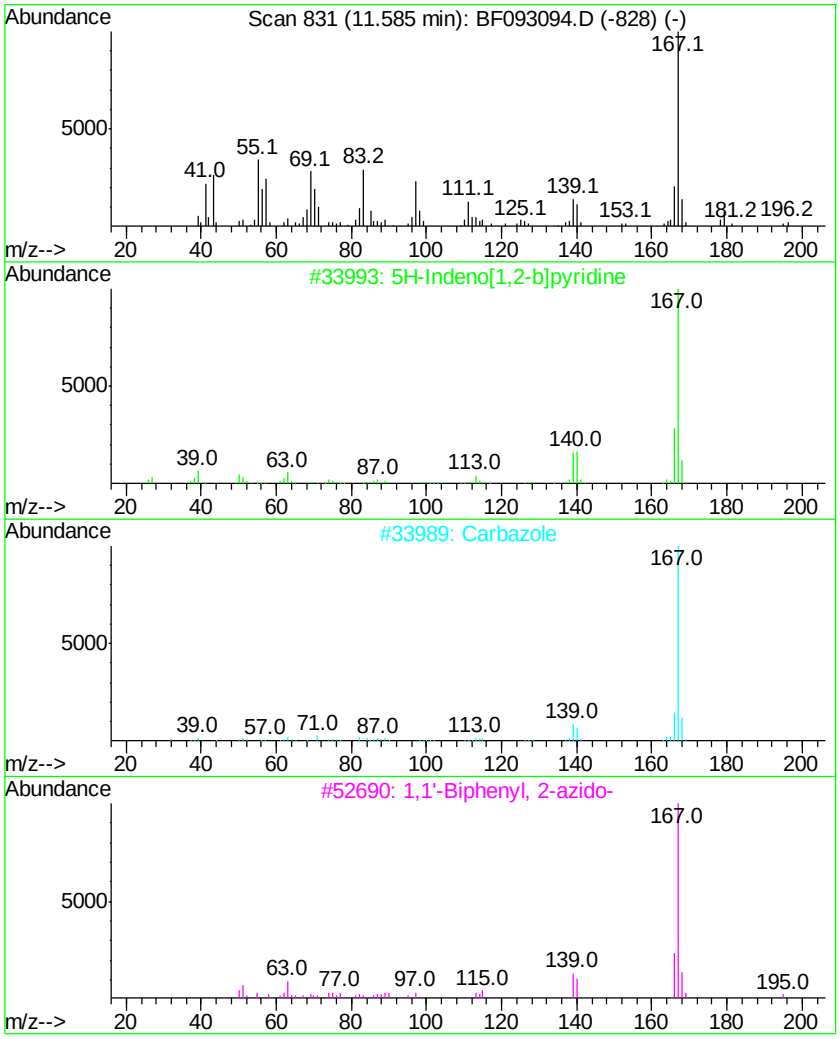
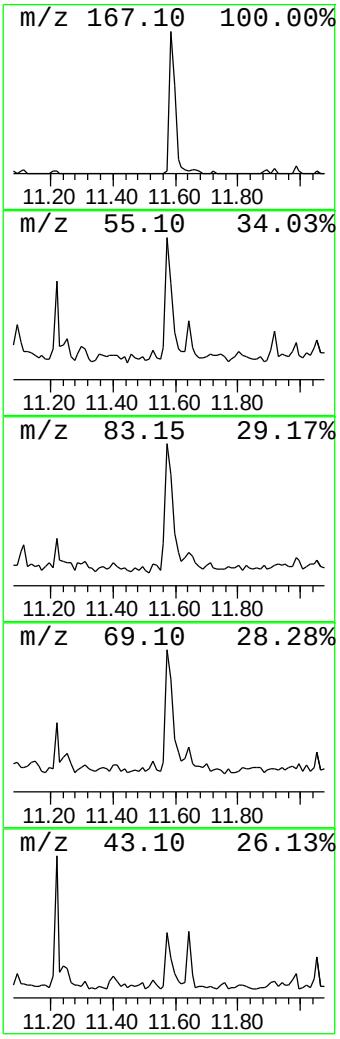
Peak Number 9 5H-Indeno[1,2-b]pyridine Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	2.94 ng	235109	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	60
2	Carbazole	167	C12H9N	000086-74-8	60
3	1,1'-Biphenyl, 2-azido-	195	C12H9N3	007599-23-7	60
4	9H-Carbazole-9-methanol	197	C13H11NO	002409-36-1	53
5	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	53





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TIC Library : C:\DATABASE\NIST02.L
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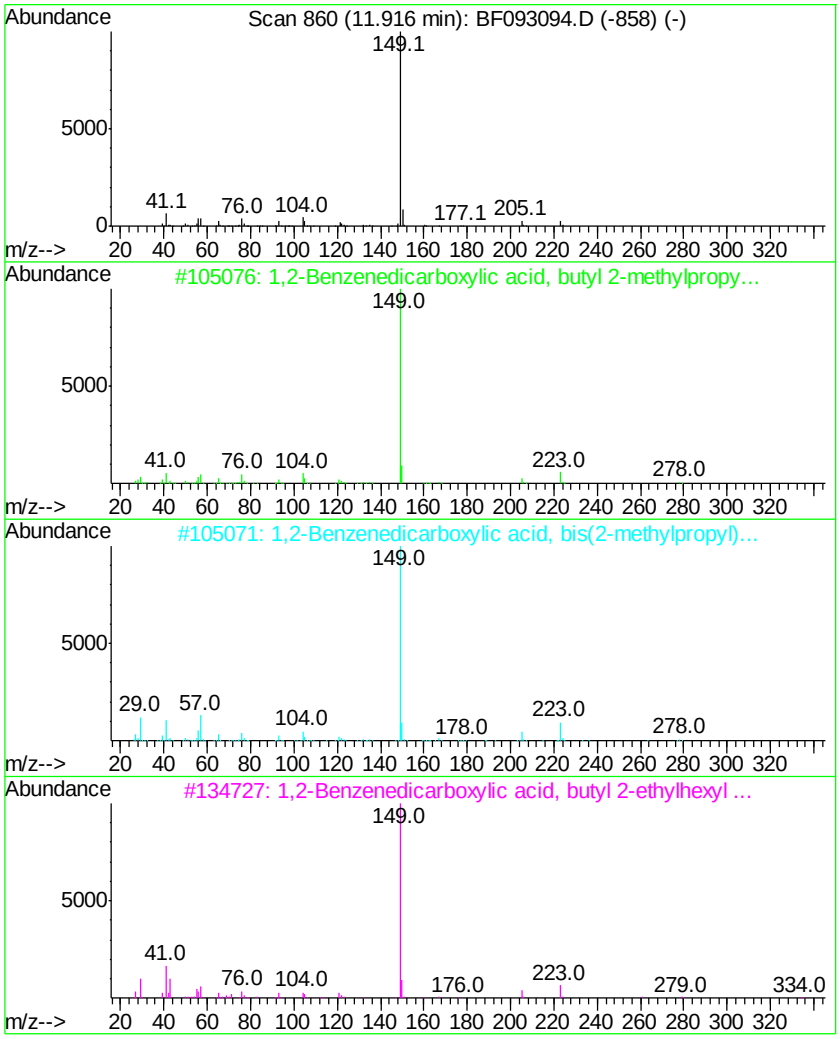
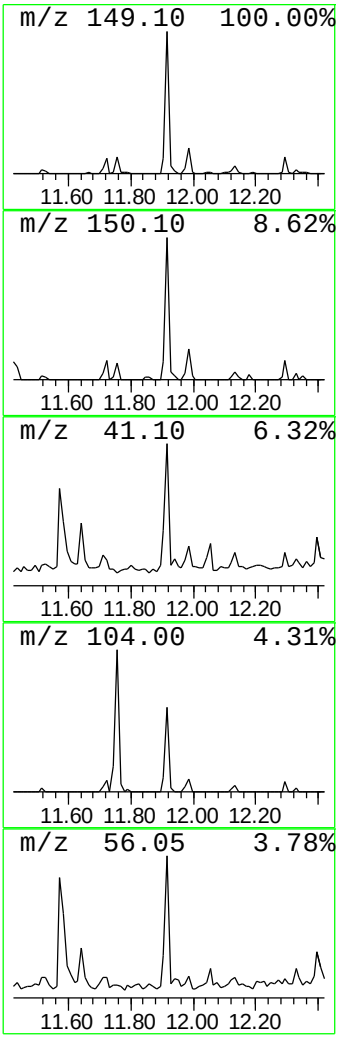
Peak Number 10 1,2-Benzenedicarboxylic aci... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.20 ng	256311	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	86
2	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	83
3	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	74
4	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	74
5	1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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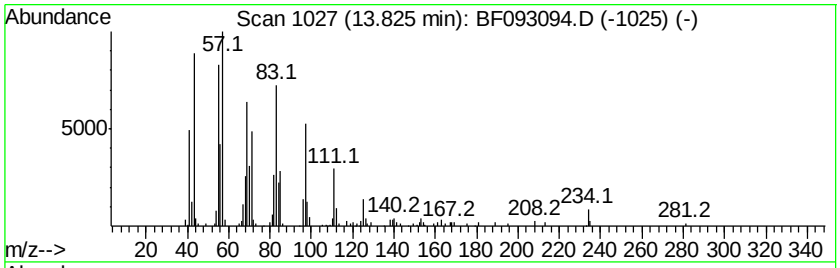
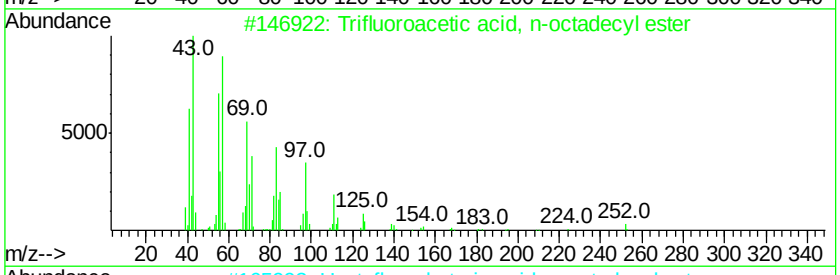
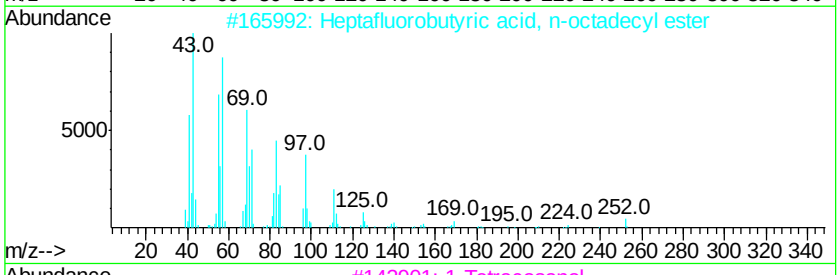
Peak Number 11 Trifluoroacetic acid, n-oct... Concentration Rank 9

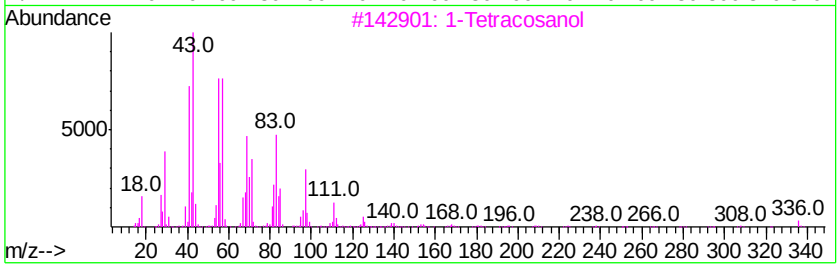
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.36 ng	272322	Chrysene-d12	13.99

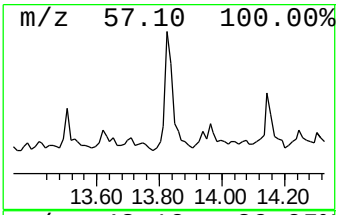
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	1-Tetracosanol	354	C24H50O	000506-51-4	91
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91

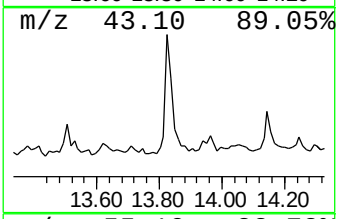


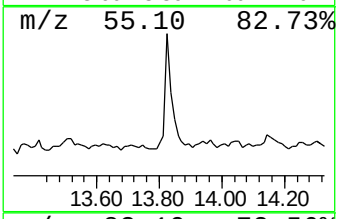


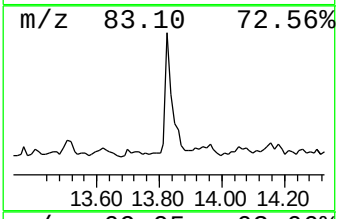


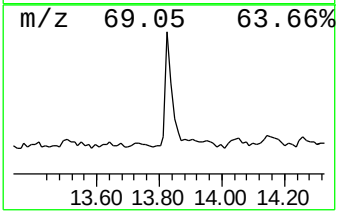












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022217\
Data File : BF093094.D
Acq On : 22 Feb 2017 23:55
Operator : SJ/MA
Sample : I1931-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-6

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one	3.09	4.7	ng	235807	1	6.84	1006270	20.0
4-Penten-2-one, 4...	3.34	16.8	ng	845768	1	6.84	1006270	20.0
3-Penten-2-one, 4...	4.40	461.9	ng	23241000	1	6.84	1006270	20.0
2-Pentanone, 4-hy...	5.06	261.1	ng	13139000	1	6.84	1006270	20.0
2-Cyclohexen-1-on...	7.16	12.3	ng	619159	1	6.84	1006270	20.0
Eicosane	10.77	3.8	ng	304718	4	11.36	1601410	20.0
5H-Indeno[1,2-b]p...	11.58	2.9	ng	235109	4	11.36	1601410	20.0
1,2-Benzenedicarb...	11.92	3.2	ng	256311	4	11.36	1601410	20.0
Trifluoroacetic a...	13.83	3.4	ng	272322	5	13.99	1622010	20.0