LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093384.D
Acq On : 4 Mar 2017 2:57
Operator : SJ/MA
Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

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	3.207	95	98	108	rVB	170163	365515	2.99%	0.742%
2	4.281	186	192	194	rBV	5581031	12220745	100.00%	24.812%
3	4.967	247	252	255	rBV	4535935	10124637	82.85%	20.556%
4	6.430	378	380	388	rBV	824597	961154	7.86%	1.951%
5	6.556	388	391	394	rVV2	191549	209040	1.71%	0.424%
6	6.784	408	411	413	rBV	982203	1217145	9.96%	2.471%
7	6.853	415	417	419	rBV	144274	158993	1.30%	0.323%
8	6.933	422	424	427	rBV	2861196	3094006	25.32%	6.282%
9	7.116	438	440	445	rBV	222114	222407	1.82%	0.452%
10	7.356	458	461	463	rBV	2903209	2857912	23.39%	5.803%
11	8.064	521	523	526	rBV	1080124	1561441	12.78%	3.170%
12	9.150	615	618	620	rBV	4306226	4477753	36.64%	9.091%
13	9.539	650	652	656	rVB	248186	295713	2.42%	0.600%
14	9.756	669	671	673	rBV	100844	123938	1.01%	0.252%
15	9.825	674	677	679	rVV	1530041	1592994	13.04%	3.234%
16	10.248	713	714	716	rVB	160884	124394	1.02%	0.253%
17	10.716	754	755	760	rVB	146888	263218	2.15%	0.534%
18	11.173	793	795	796	rBV	93450	129155	1.06%	0.262%
19	11.310	804	807	808	rBV	1030702	1437813	11.77%	2.919%
20	11.871	854	856	858	rBV	337800	466425	3.82%	0.947%
21	11.928	858	861	864	rVB2	112151	174647	1.43%	0.355%
22	12.522	911	913	915	rBV	165776	209087	1.71%	0.425%
23	12.751	930	933	936	rBV	138314	201384	1.65%	0.409%
24	12.888	942	945	948	rBV	3110889	2999921	24.55%	6.091%
25	13.779	1020	1023	1029	rVB2	196058	298770	2.44%	0.607%
26	13.939	1035	1037	1043	rVB	1001980	1168582	9.56%	2.373%
27	14.408	1076	1078	1083	rBV3	67756	160118	1.31%	0.325%
28	15.002	1128	1130	1133	rVB	76173	127651	1.04%	0.259%
29	15.357	1158	1161	1164	rBV	869007	1088374	8.91%	2.210%
30	15.757	1193	1196	1198	rBV	132763	195375	1.60%	0.397%
31	16.214	1233	1236	1241	rVB	134491	250203	2.05%	0.508%
32	16.751	1280	1283	1288	rVB	119345	266351	2.18%	0.541%
33	17.380	1335	1338	1343	rVB3	80395	208161	1.70%	0.423%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093384.D
Acq On : 4 Mar 2017 2:57
Operator : SJ/MA
Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

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

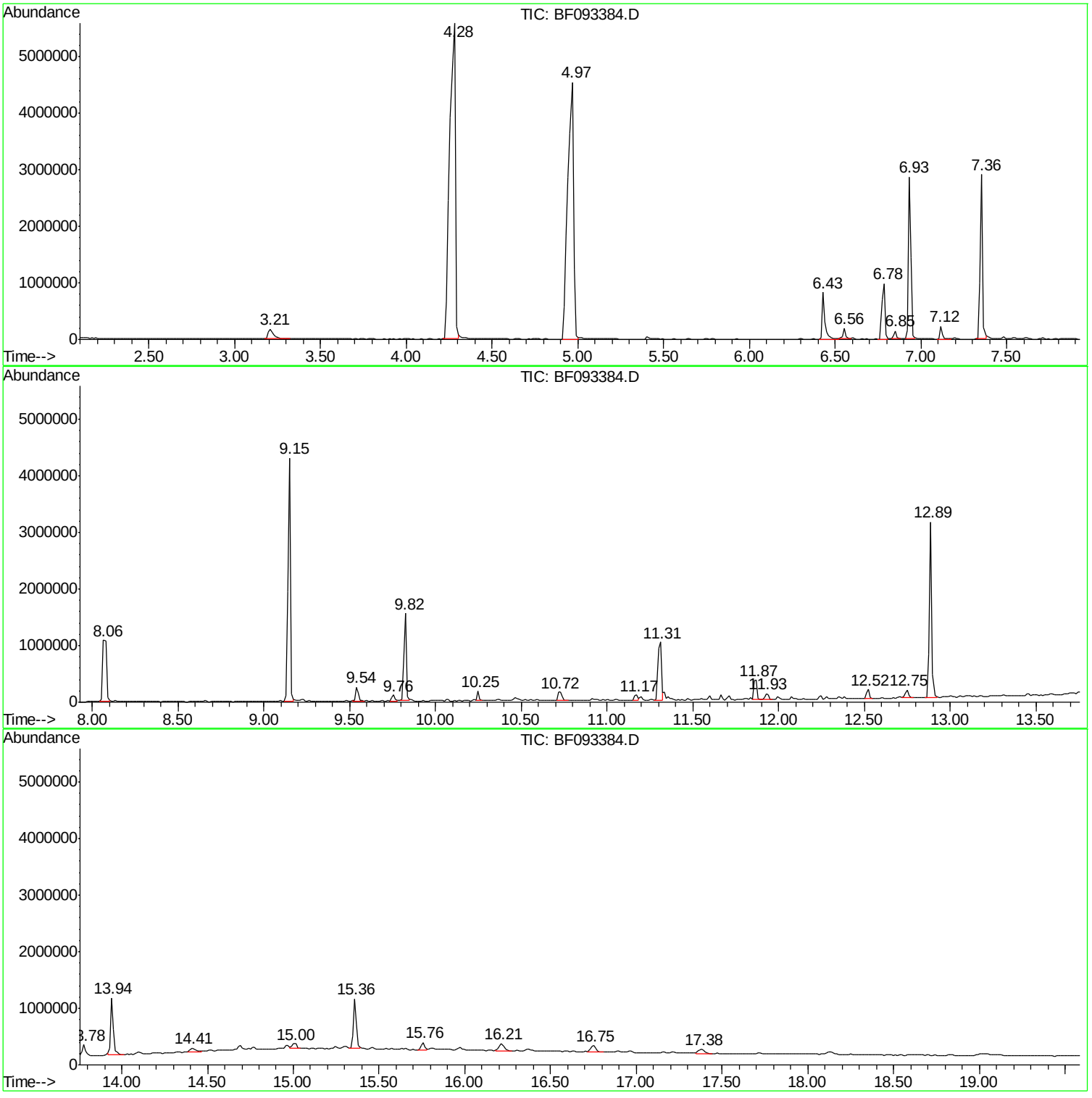
Sum of corrected areas: 49253022

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093384.D
Acq On : 4 Mar 2017 2:57
Operator : SJ/MA
Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-7

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

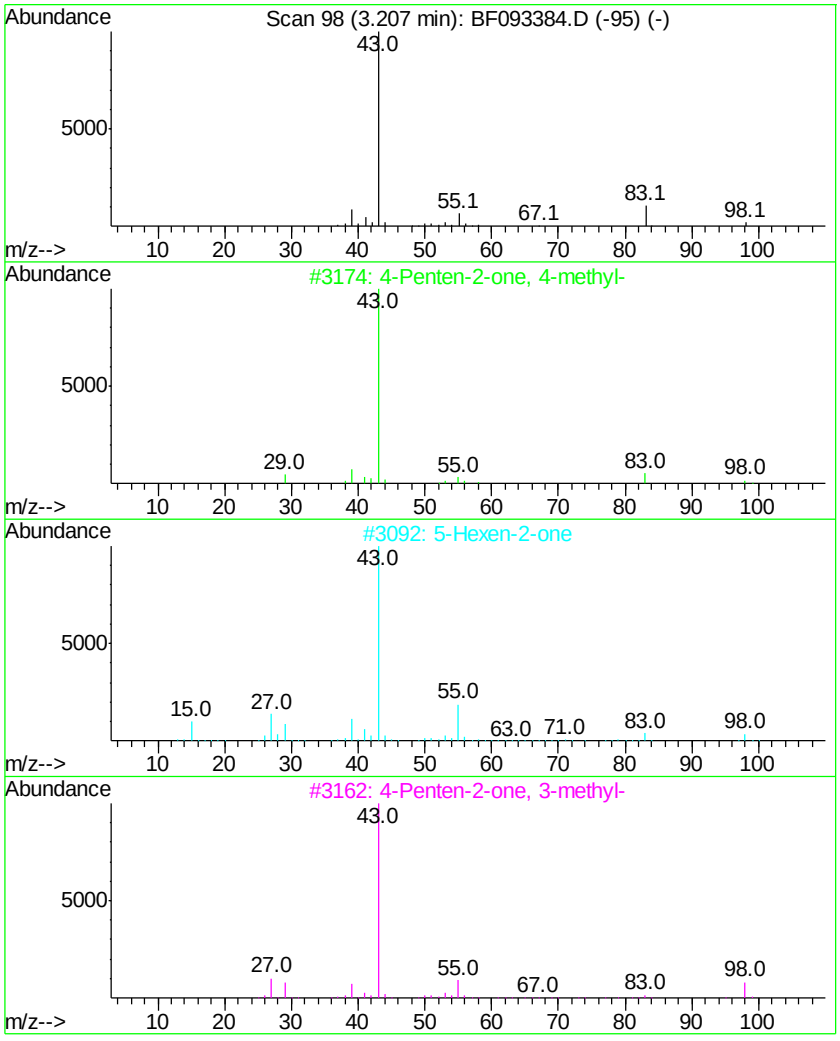
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

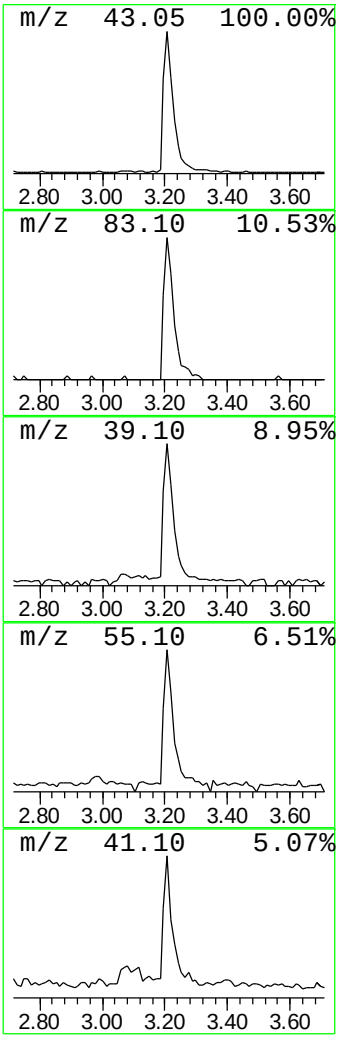
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	6.01 ng	365515	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	38
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	33
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	30
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093384.D
Acq On : 4 Mar 2017 2:57
Operator : SJ/MA
Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

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

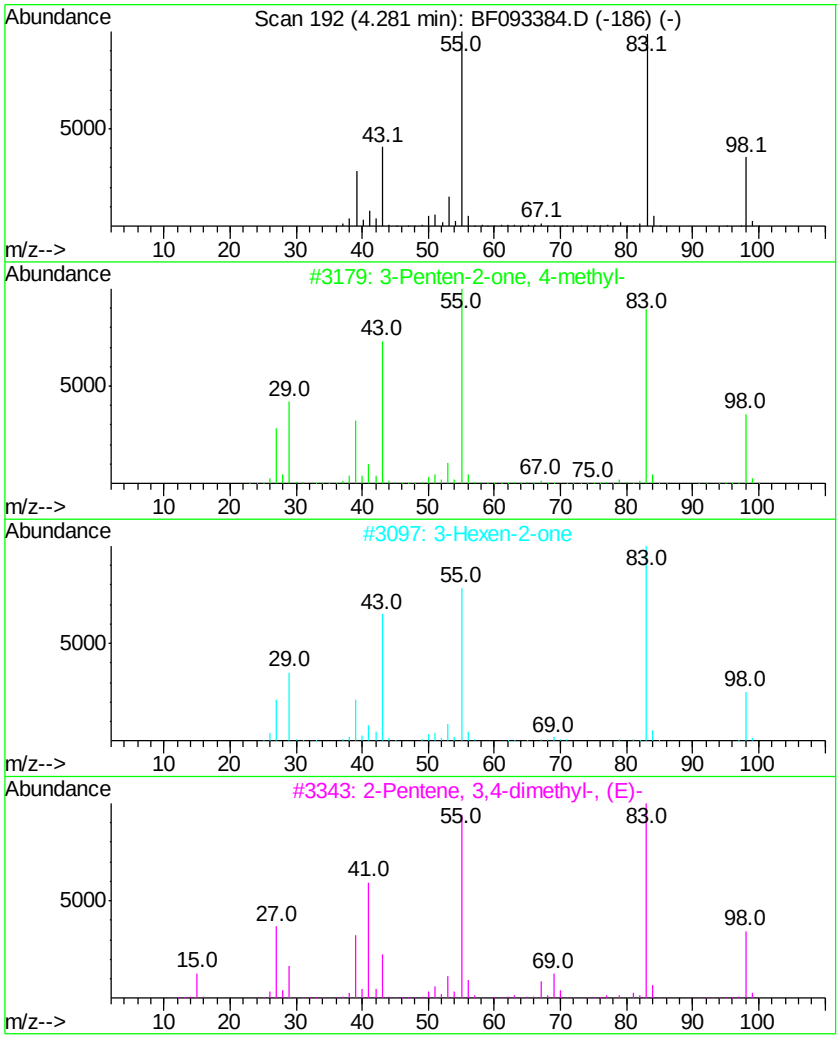
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

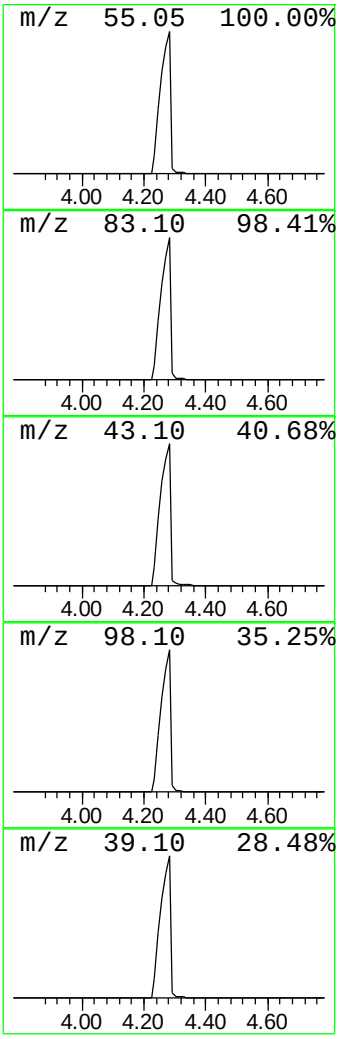
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	200.81 ng	12220700	1,4-Dichlorobenzene-d4	6.78

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, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
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Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

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

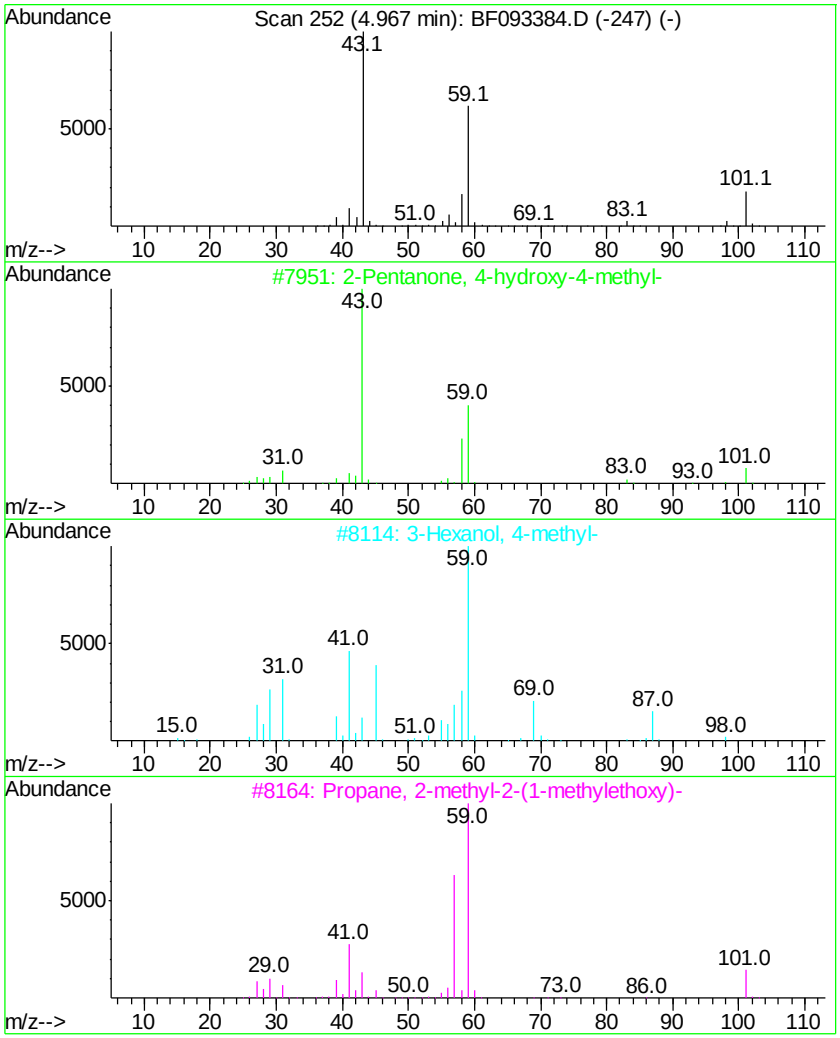
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

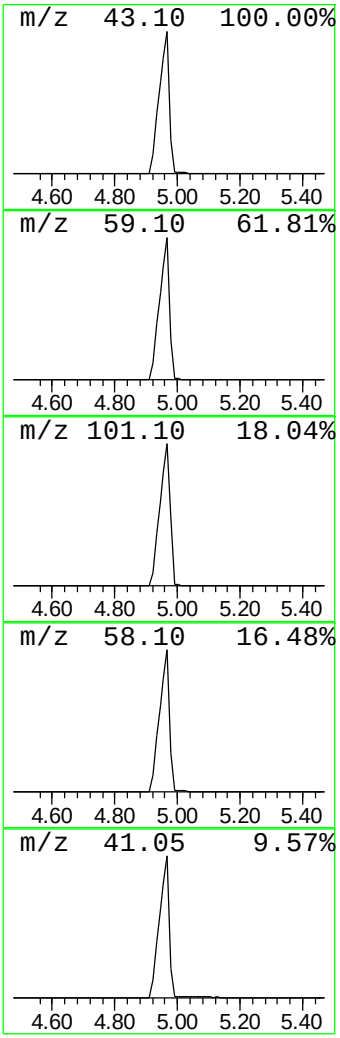
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	166.37 ng	10124600	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
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Sample : I2078-13
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Instrument : BNA_F
ClientSampleId : C-7

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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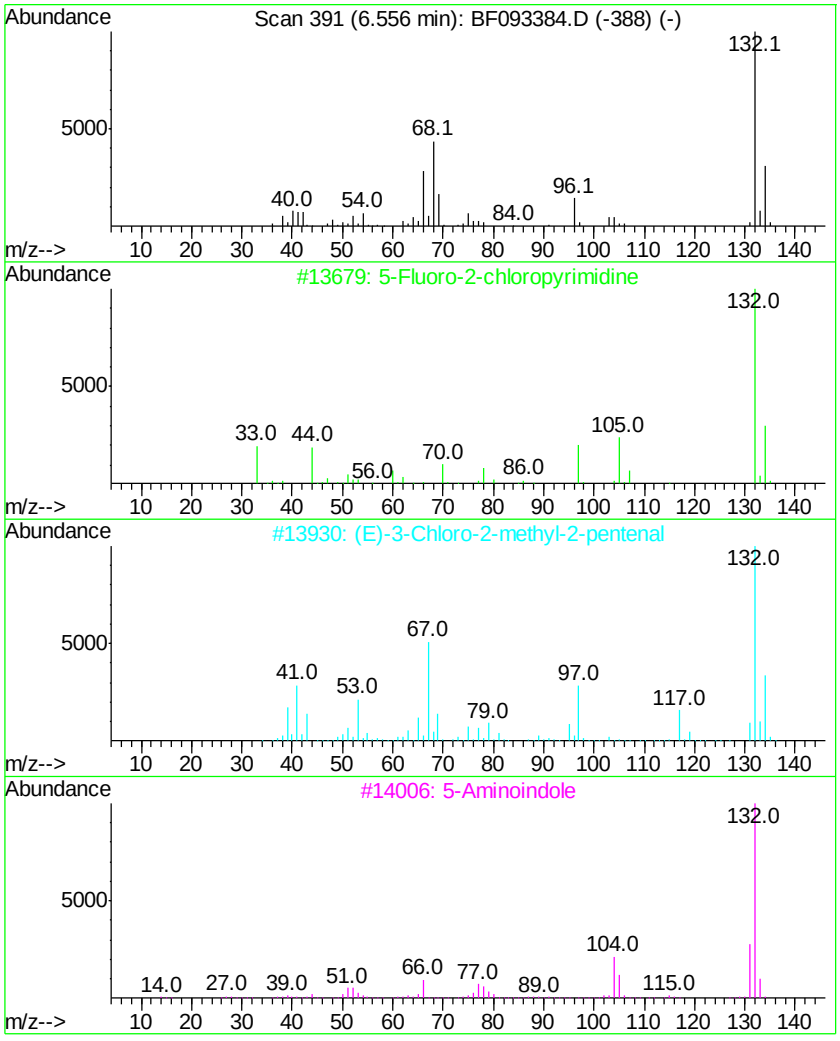
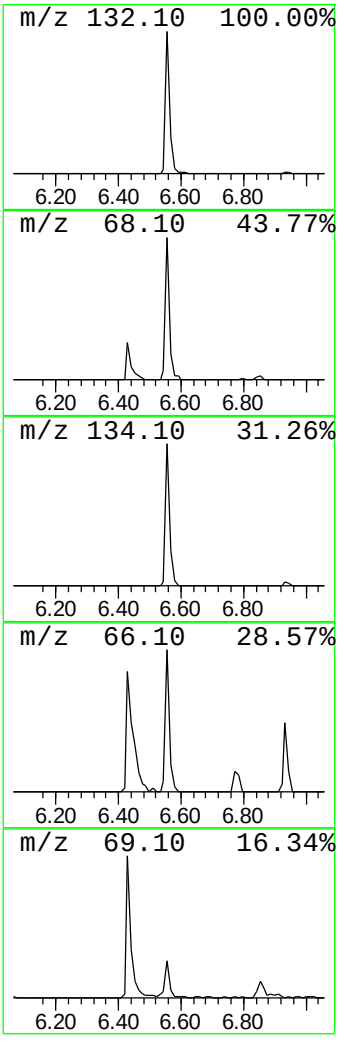
Peak Number 4 unknown6.56 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	3.43 ng	209040	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

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

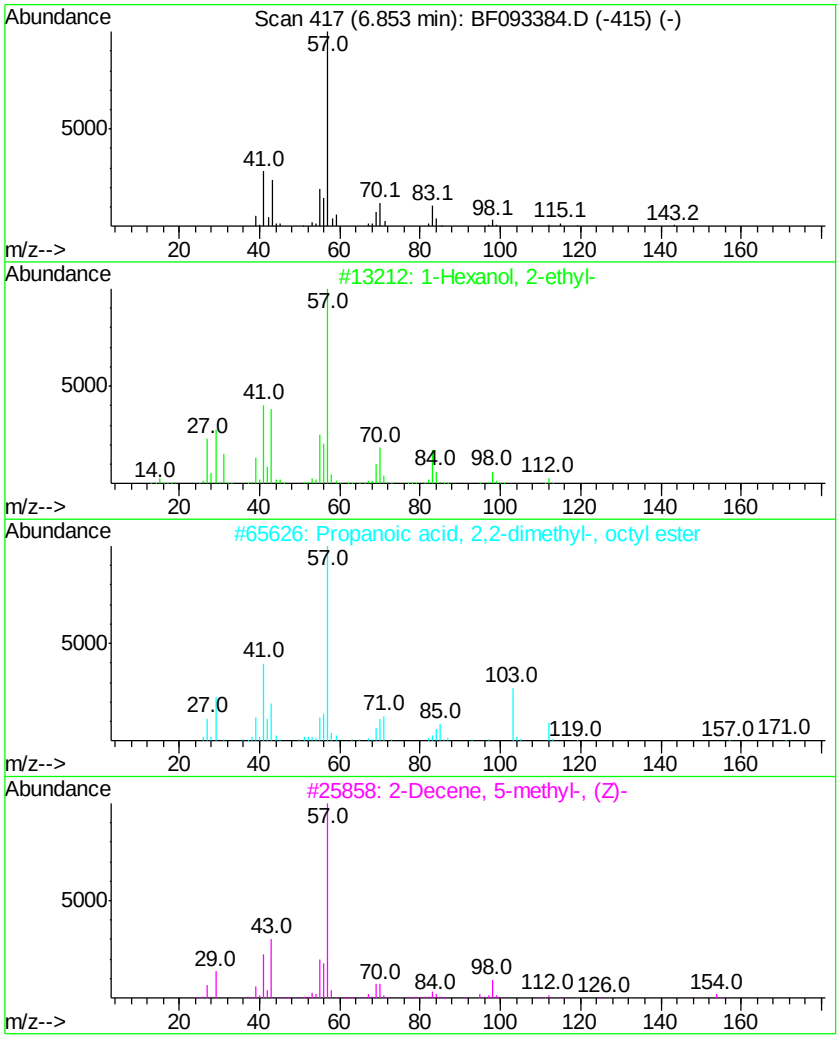
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

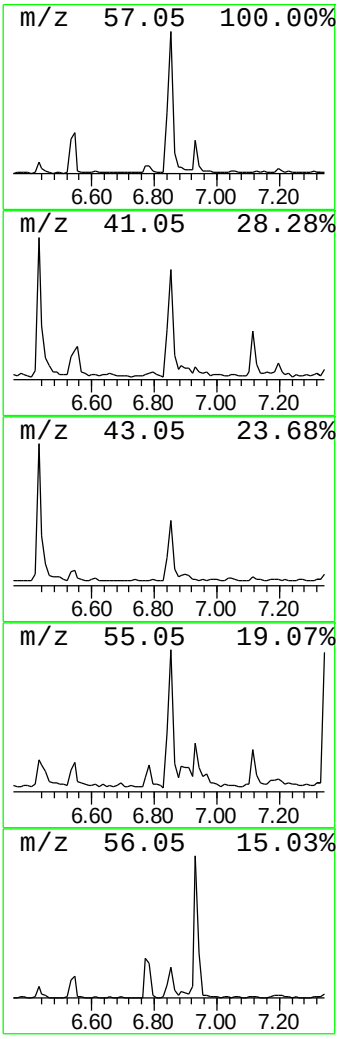
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.85	2.61 ng	158993	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	64
3	2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	53
4	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47





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Sample : I2078-13
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Instrument : BNA_F
ClientSampleId : C-7

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

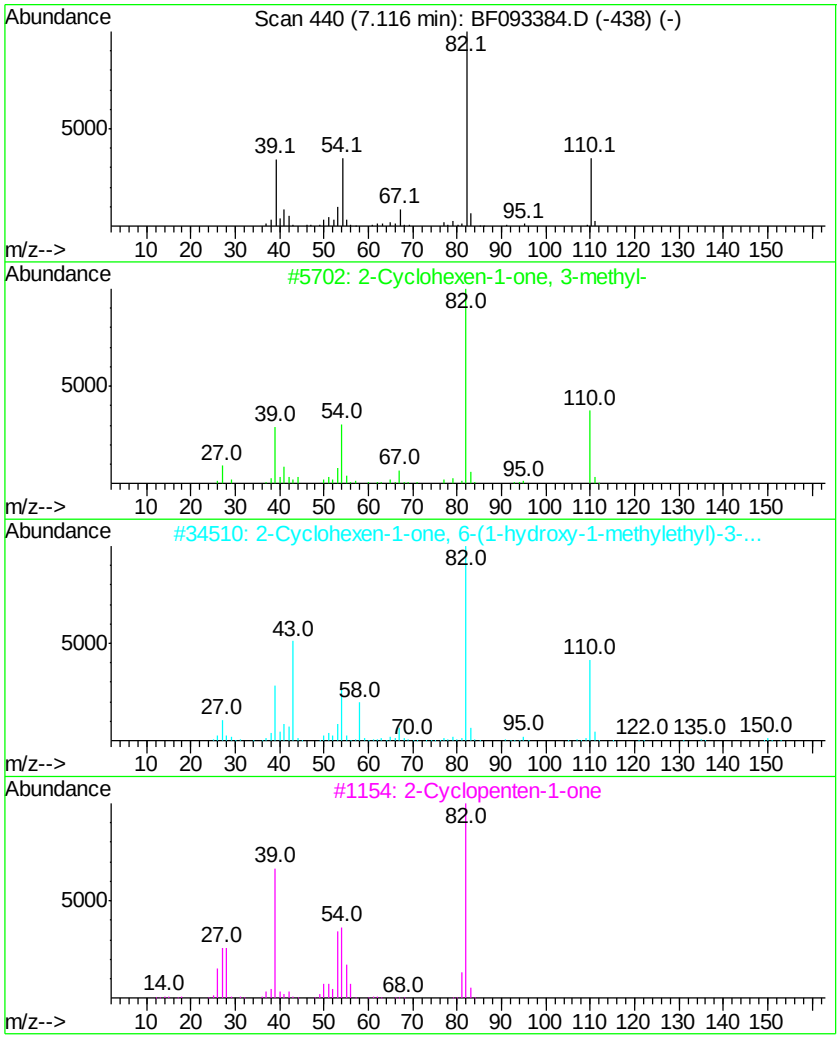
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

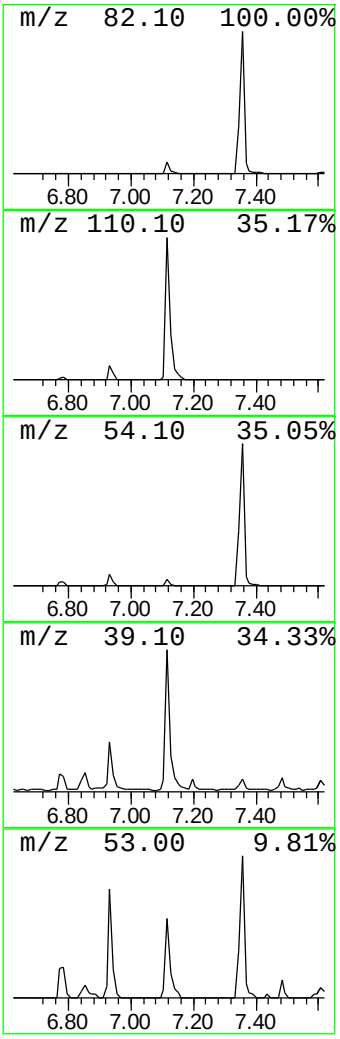
****

Peak Number 7 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	3.65 ng	222407	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	64
3	2-Cyclopenten-1-one	82	C5H6O	000930-30-3	53
4	Betazole	111	C5H9N3	000105-20-4	49
5	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	45





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Sample : I2078-13
Misc :
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Instrument : BNA_F
ClientSampleId : C-7

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

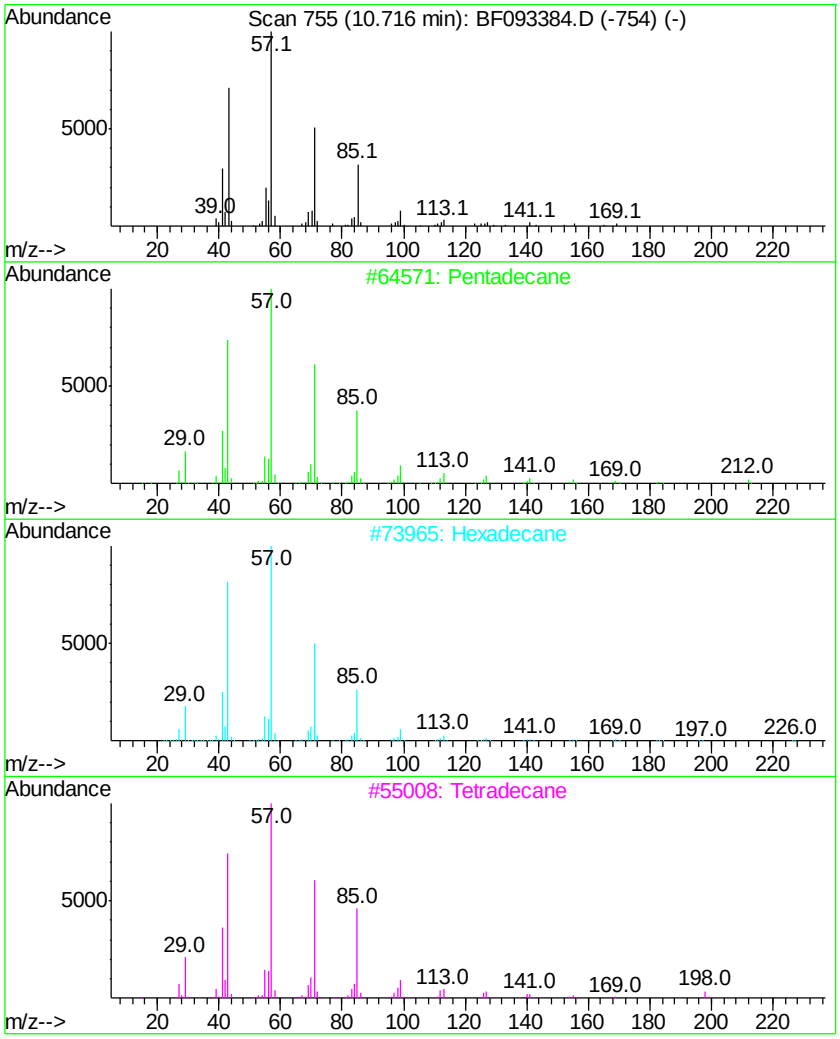
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

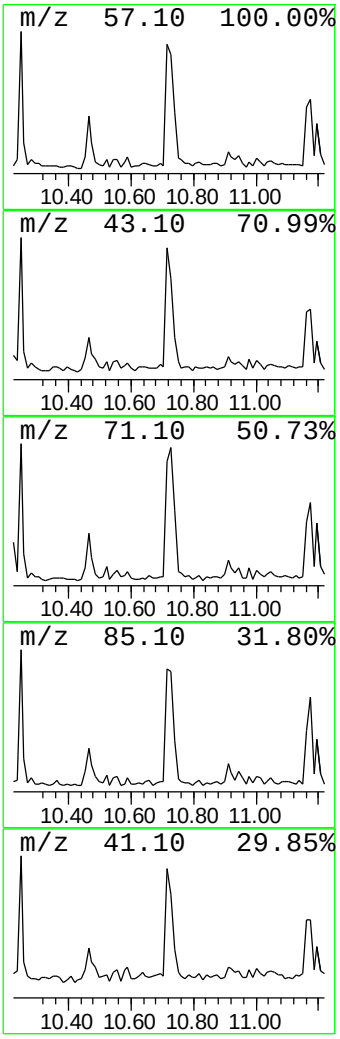
****

Peak Number 8 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	3.66 ng	263218	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hexadecane	226	C16H34	000544-76-3	87
3	Tetradecane	198	C14H30	000629-59-4	86
4	Tridecane	184	C13H28	000629-50-5	78
5	Heptadecane	240	C17H36	000629-78-7	72





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Instrument : BNA_F
ClientSampleId : C-7

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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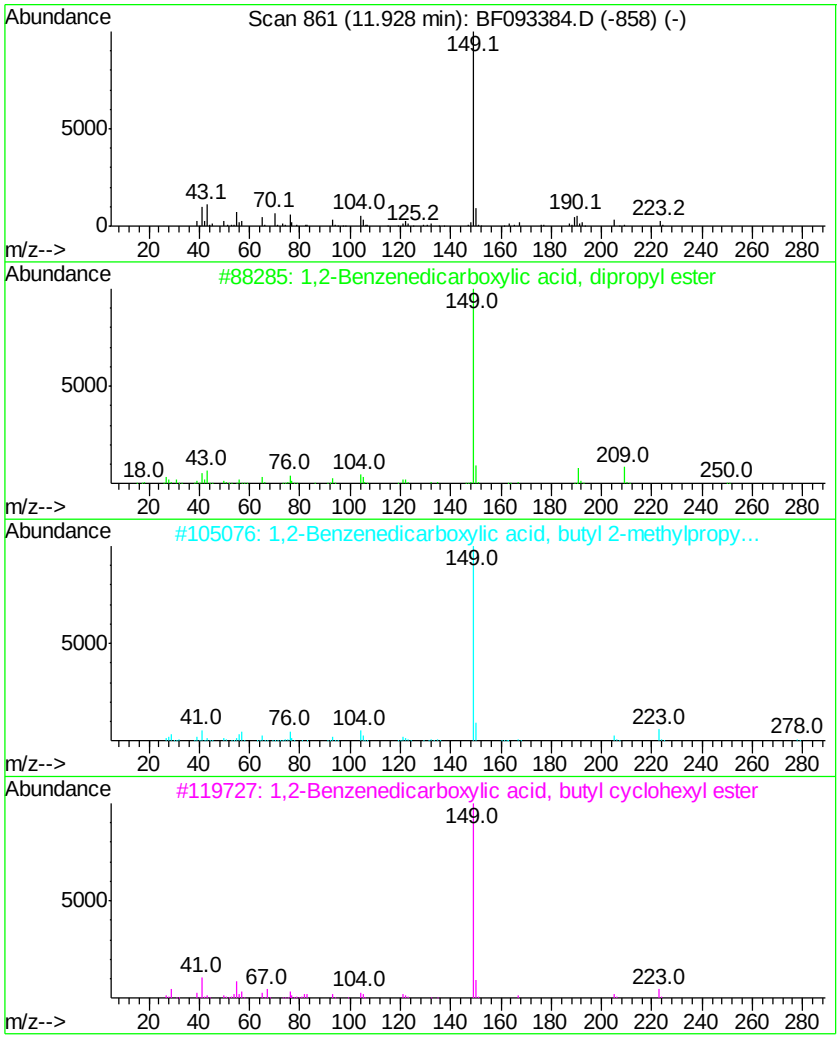
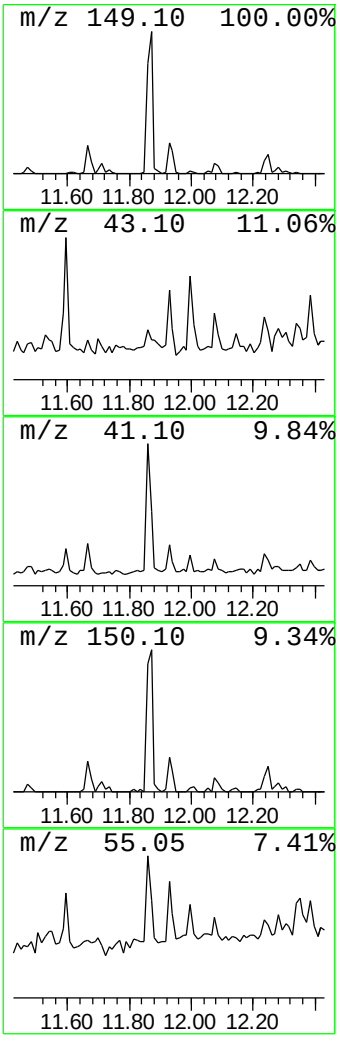
Peak Number 9 1,2-Benzenedicarboxylic aci... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.43 ng	174647	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	80
2	1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	72
3	1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	72
4	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	72
5	Dibutyl phthalate	278	C16H22O4	000084-74-2	56





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093384.D
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Operator : SJ/MA
Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

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

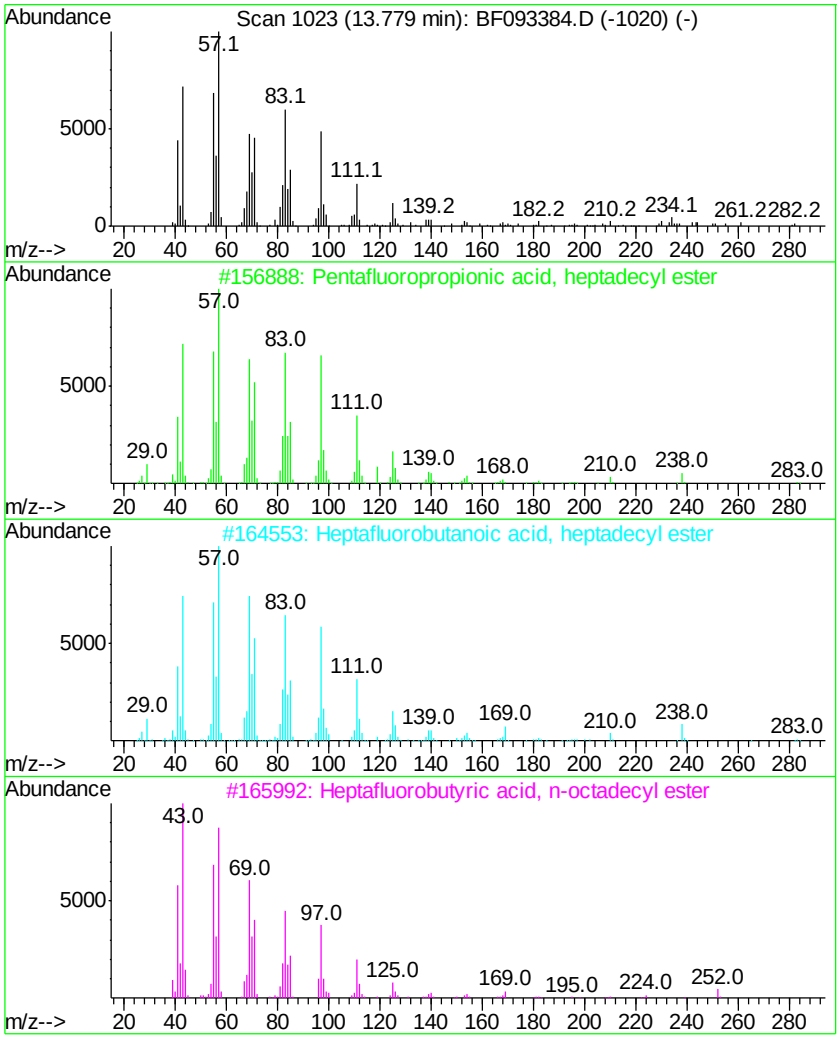
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

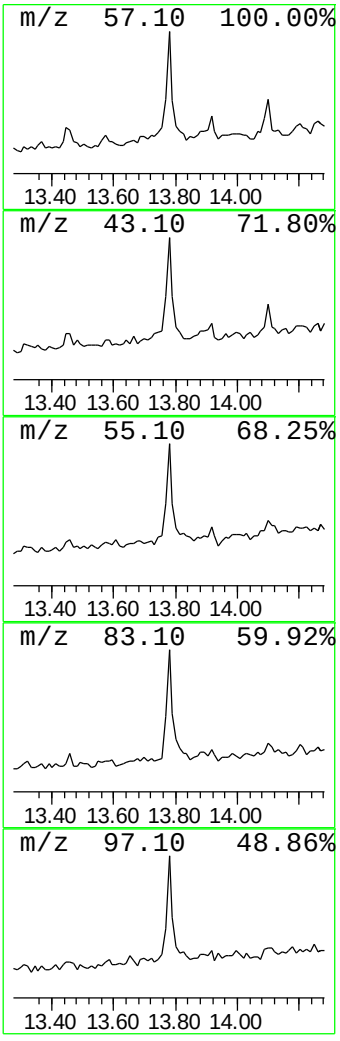
****

Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	5.11 ng	298770	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87





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Acq On : 4 Mar 2017 2:57
Operator : SJ/MA
Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

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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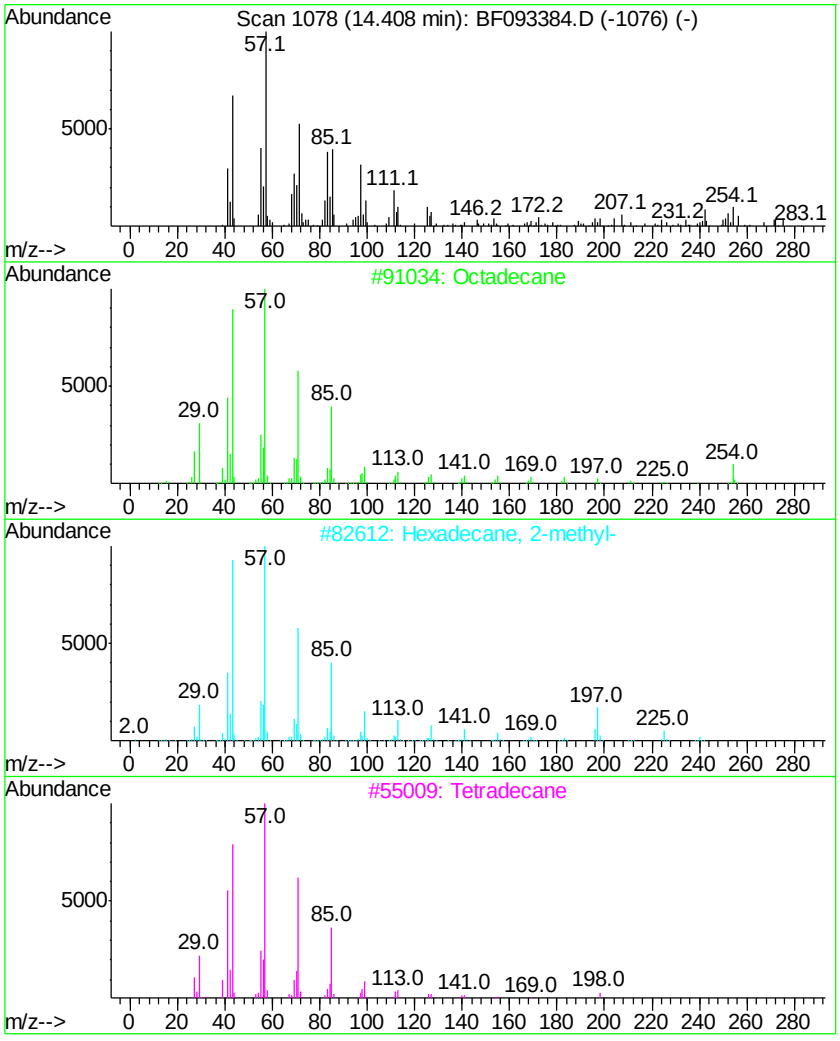
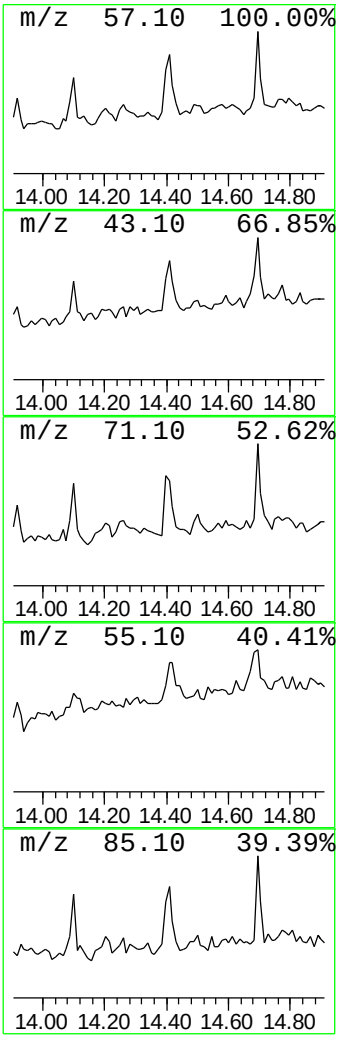
Peak Number 11 Octadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	2.74 ng	160118	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	83
2	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	60
3	Tetradecane	198	C14H30	000629-59-4	60
4	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	58
5	Undecane, 2-methyl-	170	C12H26	007045-71-8	55





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Operator : SJ/MA
Sample : I2078-13
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ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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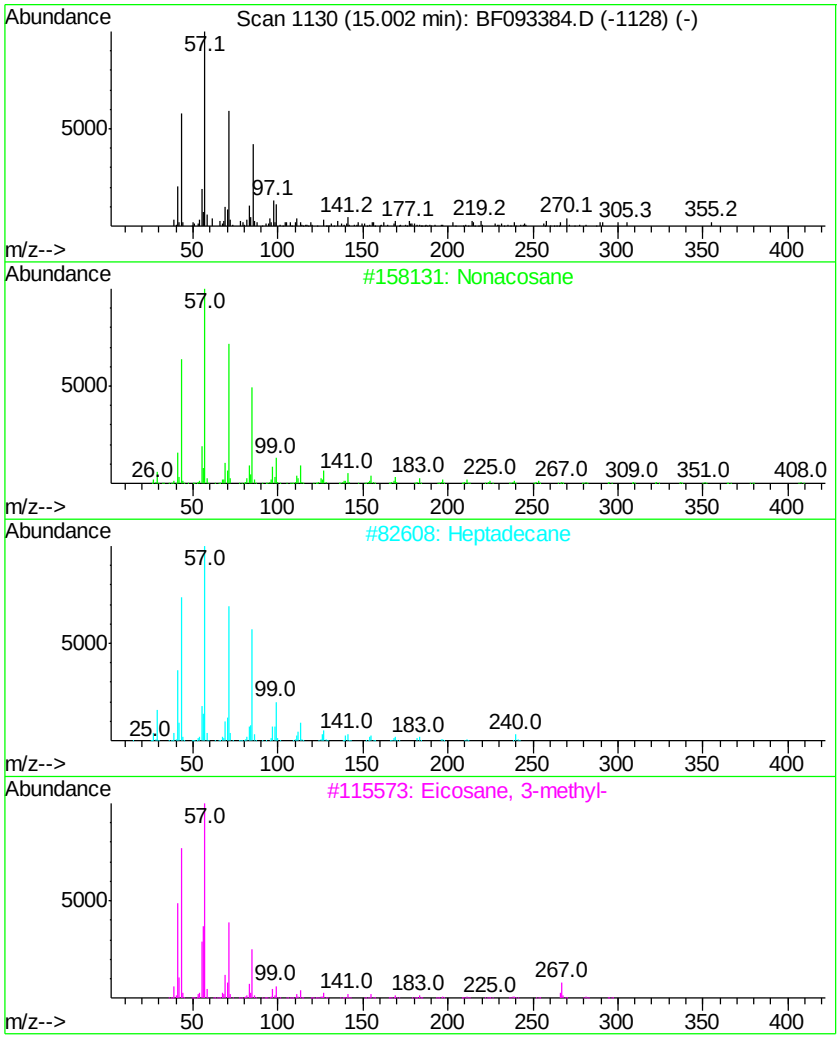
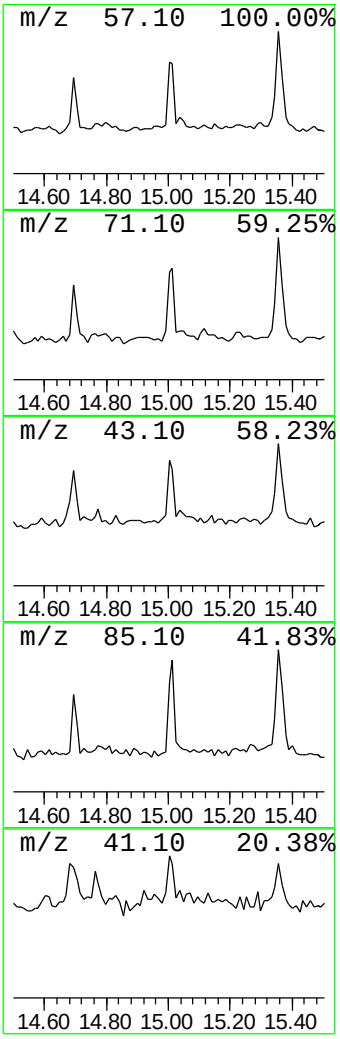
Peak Number 12 Nonacosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.35 ng	127651	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosane	408	C29H60	000630-03-5	86
2	Heptadecane	240	C17H36	000629-78-7	80
3	Eicosane, 3-methyl-	296	C21H44	006418-46-8	78
4	Hexacosane	366	C26H54	000630-01-3	78
5	Tetratetracontane	619	C44H90	007098-22-8	78





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Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
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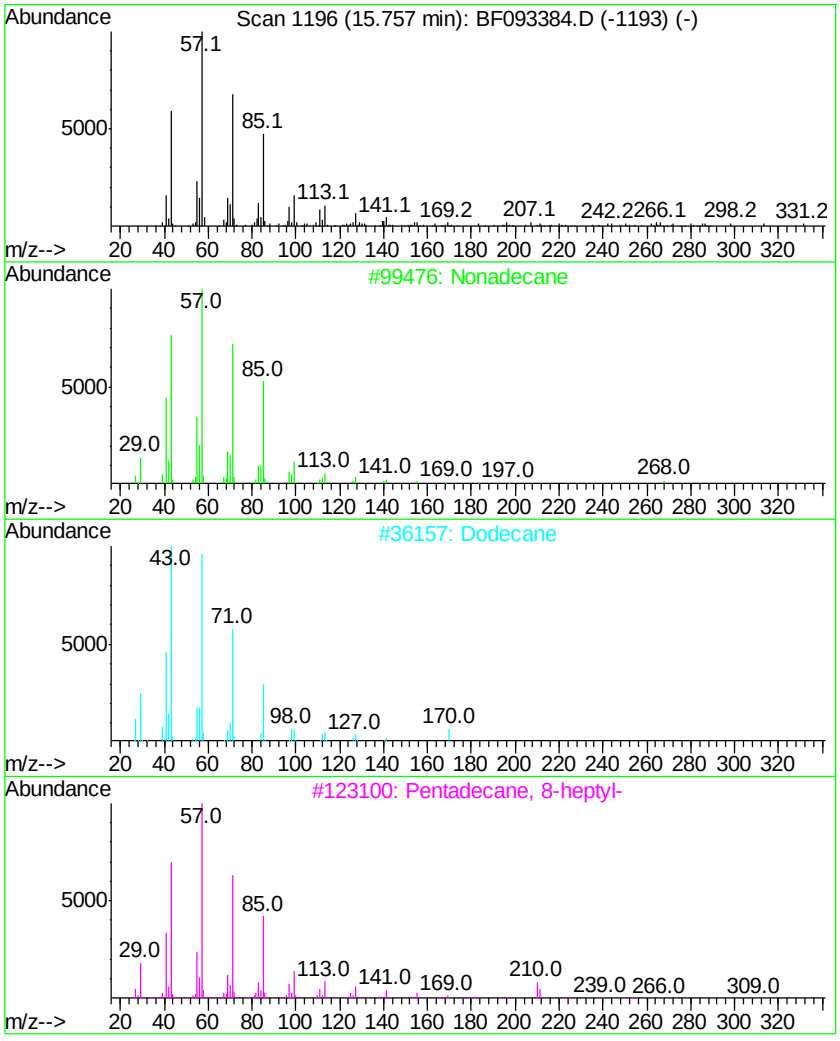
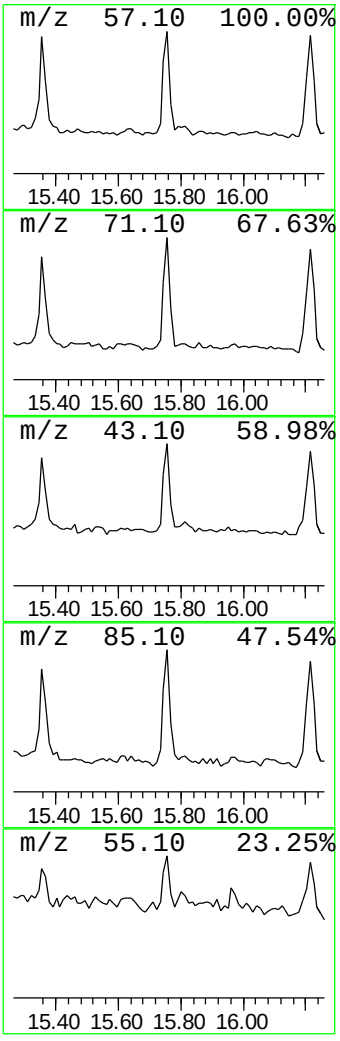
Peak Number 13 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	3.59 ng	195375	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	87
2	Dodecane	170	C12H26	000112-40-3	87
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
4	Docosane, 9-butyl-	366	C26H54	055282-14-9	86
5	Tetracosane	338	C24H50	000646-31-1	86





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Operator : SJ/MA
Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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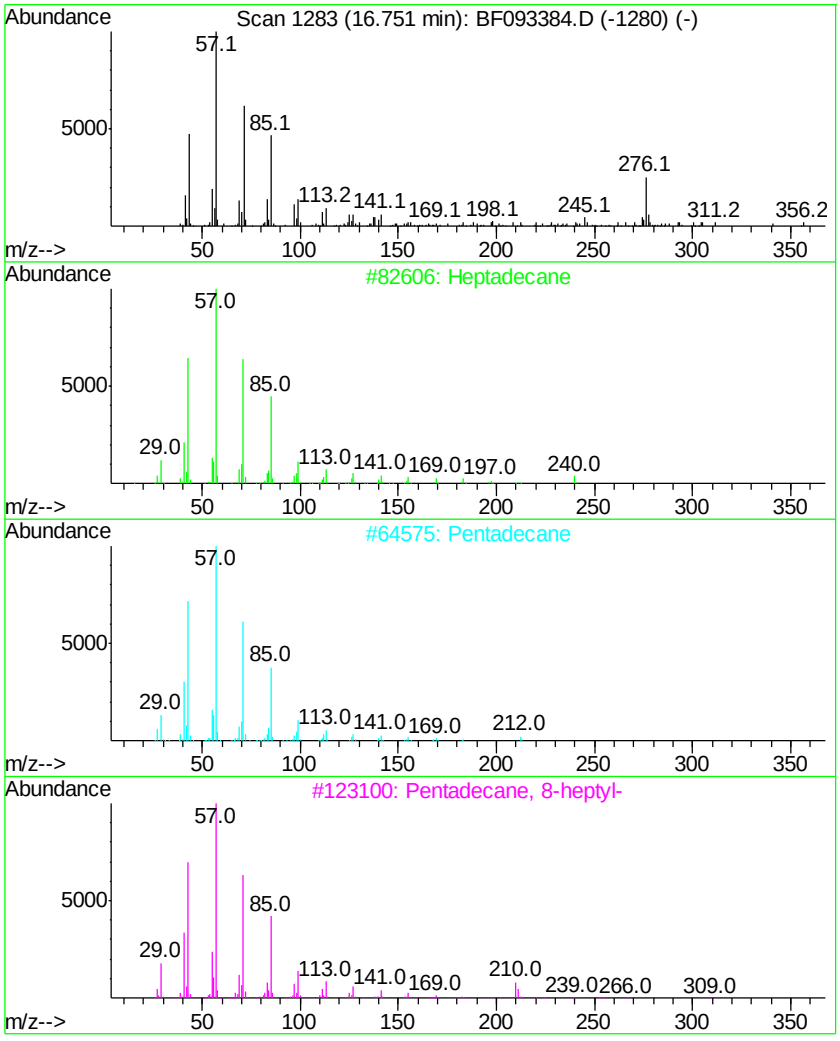
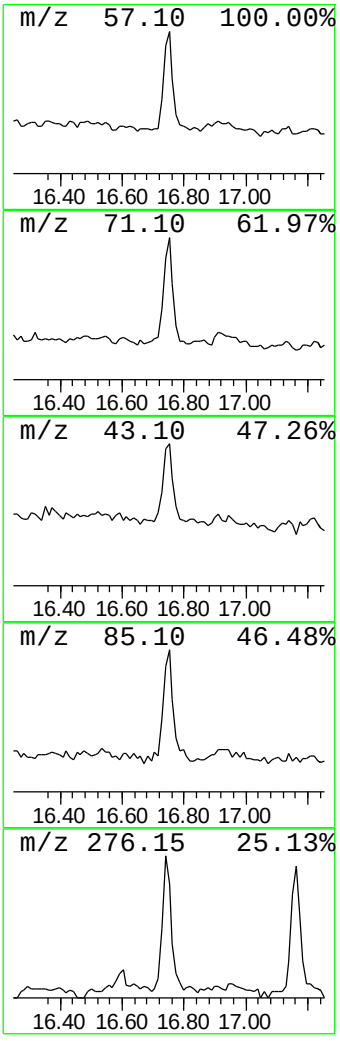
Peak Number 15 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	4.89 ng	266351	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	76
2	Pentadecane	212	C15H32	000629-62-9	70
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	68
4	Nonacosane	408	C29H60	000630-03-5	64
5	Eicosane	282	C20H42	000112-95-8	62





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Acq On : 4 Mar 2017 2:57
Operator : SJ/MA
Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

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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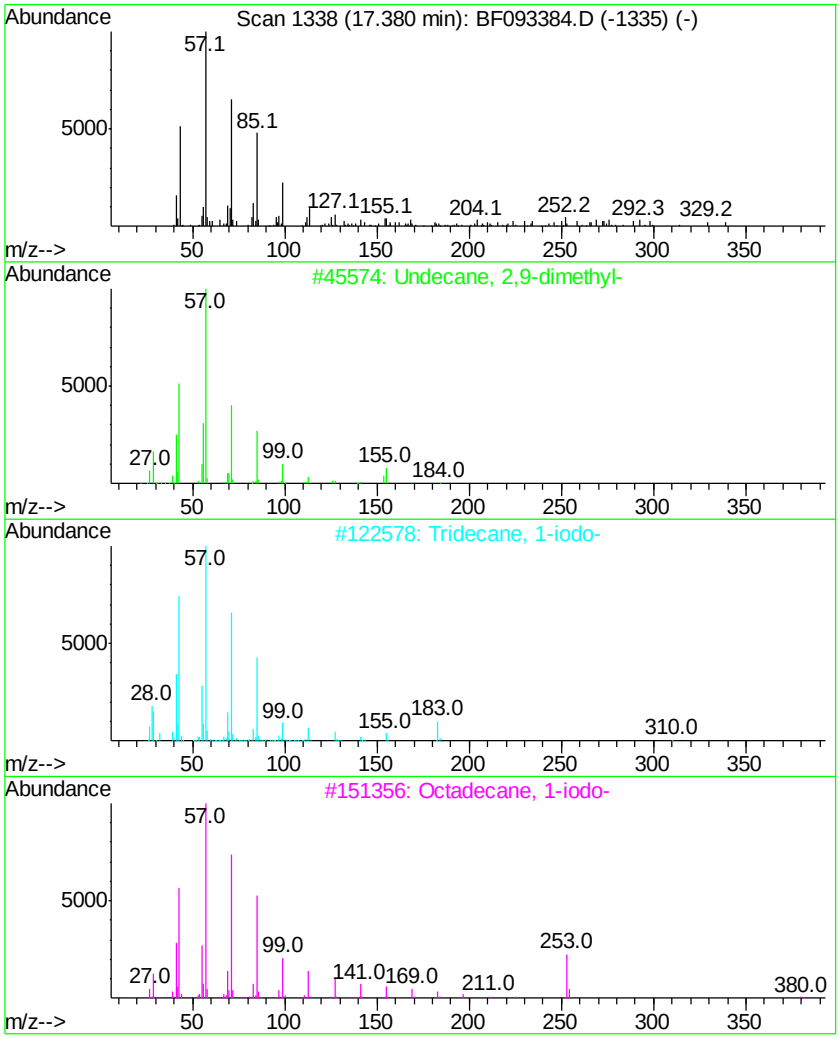
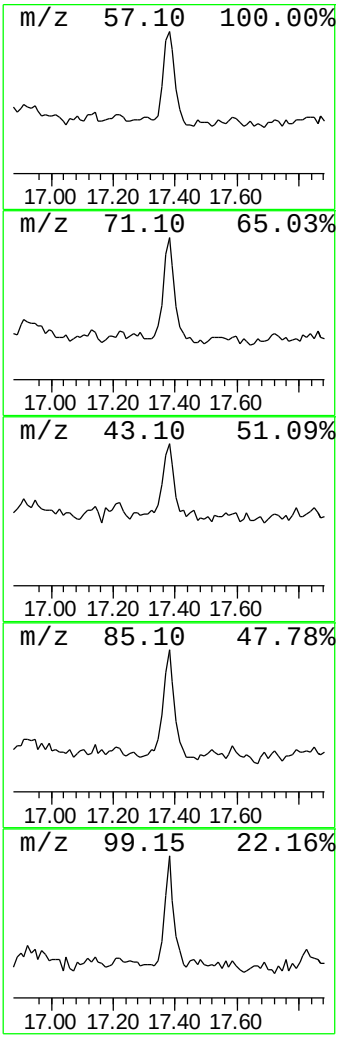
Peak Number 16 Undecane, 2,9-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	3.83 ng	208161	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	86
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
4	Nonadecane	268	C19H40	000629-92-5	72
5	Heptadecane	240	C17H36	000629-78-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030317\
Data File : BF093384.D
Acq On : 4 Mar 2017 2:57
Operator : SJ/MA
Sample : I2078-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-7

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
4-Penten-2-one, 4...	3.21	6.0	ng	365515	1	6.78	1217150	20.0
3-Penten-2-one, 4...	4.28	200.8	ng	12220700	1	6.78	1217150	20.0
2-Pentanone, 4-hy...	4.97	166.4	ng	10124600	1	6.78	1217150	20.0
unknown6.56	6.56	3.4	ng	209040	1	6.78	1217150	20.0
1-Hexanol, 2-ethyl-	6.85	2.6	ng	158993	1	6.78	1217150	20.0
2-Cyclohexen-1-on...	7.12	3.6	ng	222407	1	6.78	1217150	20.0
Pentadecane	10.72	3.7	ng	263218	4	11.31	1437810	20.0
1,2-Benzenedicarb...	11.93	2.4	ng	174647	4	11.31	1437810	20.0
Pentafluoropropio...	13.78	5.1	ng	298770	5	13.94	1168580	20.0
Octadecane	14.41	2.7	ng	160118	5	13.94	1168580	20.0
Nonacosane	15.00	2.4	ng	127651	6	15.36	1088370	20.0
Nonadecane	15.76	3.6	ng	195375	6	15.36	1088370	20.0
Heptadecane	16.75	4.9	ng	266351	6	15.36	1088370	20.0
Undecane, 2,9-dim...	17.38	3.8	ng	208161	6	15.36	1088370	20.0