LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093379.D
Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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	94	98	109	rVB	105814	244360	2.68%	0.507%
2	4.270	186	191	193	rBV	4968429	9128235	100.00%	18.929%
3	4.956	246	251	253	rBV	3781734	6584395	72.13%	13.654%
4	5.390	287	289	297	rBV	276253	435101	4.77%	0.902%
5	6.430	378	380	388	rBV	2471529	2510155	27.50%	5.205%
6	6.556	388	391	393	rVV	871433	934949	10.24%	1.939%
7	6.784	409	411	413	rBV	1229771	1243528	13.62%	2.579%
8	6.853	414	417	419	rBV	135400	130888	1.43%	0.271%
9	6.944	422	425	427	rBV	2825456	3907390	42.81%	8.103%
10	7.116	438	440	444	rBV	176330	212110	2.32%	0.440%
11	7.356	459	461	464	rBV	2824712	3139007	34.39%	6.509%
12	7.836	500	503	514	rVB	52060	106694	1.17%	0.221%
13	8.076	521	524	526	rBV	1809112	1733412	18.99%	3.595%
14	9.150	615	618	620	rBV	4973207	4819098	52.79%	9.993%
15	9.550	650	653	655	rBV	343597	480198	5.26%	0.996%
16	9.756	669	671	673	rBV	127682	141577	1.55%	0.294%
17	9.825	674	677	679	rVV	1811718	1692421	18.54%	3.510%
18	10.248	713	714	716	rVB	192931	153755	1.68%	0.319%
19	10.465	730	733	737	rBV	65186	113100	1.24%	0.235%
20	10.716	753	755	760	rVB	202355	319022	3.49%	0.662%
21	11.162	793	794	796	rBV	137701	186270	2.04%	0.386%
22	11.299	804	806	810	rBV	1325339	1828875	20.04%	3.793%
23	11.596	830	832	834	rBV	100709	118762	1.30%	0.246%
24	11.859	854	855	858	rVB	156776	165122	1.81%	0.342%
25	11.928	858	861	864	rVB3	60156	111210	1.22%	0.231%
26	12.511	911	912	915	rBV	143415	211958	2.32%	0.440%
27	12.739	930	932	936	rVV	126467	217902	2.39%	0.452%
28	12.888	942	945	948	rBV	3907807	4014743	43.98%	8.325%
29	13.779	1021	1023	1029	rVB2	249912	376654	4.13%	0.781%
30	13.939	1035	1037	1044	rVB	1209087	1268092	13.89%	2.630%
31	14.408	1076	1078	1080	rBV2	71405	119352	1.31%	0.248%
32	14.762	1107	1109	1112	rVB2	85446	105701	1.16%	0.219%
33	15.357	1158	1161	1167	rVB	866802	1169156	12.81%	2.425%
34	16.214	1234	1236	1240	rVB2	78787	144709	1.59%	0.300%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093379.D
Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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

35	16.740	1280	1282	1287	rBV	75040	154455	1.69%	0.320%

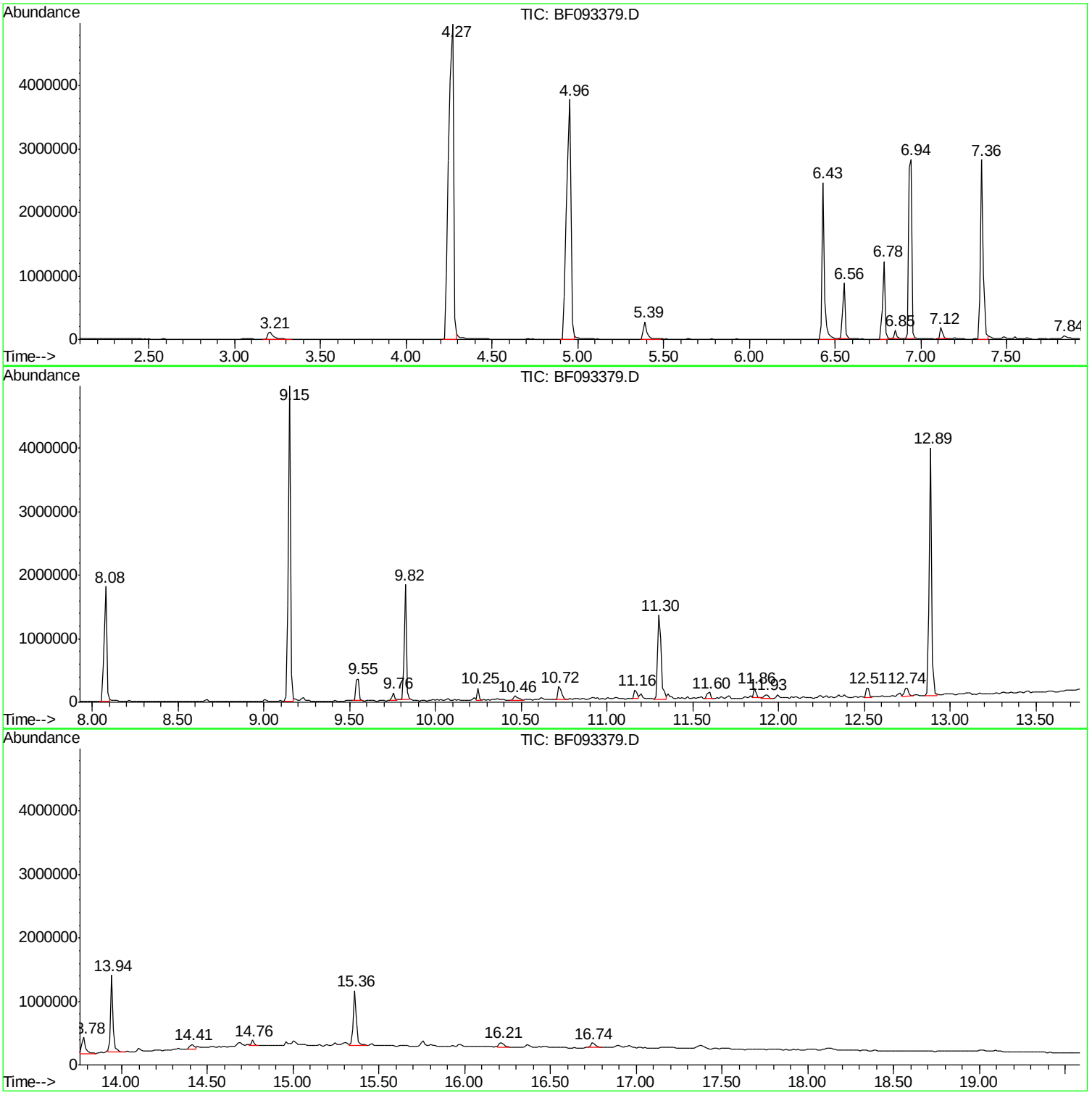
Sum of corrected areas: 48222356

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093379.D
Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093379.D
Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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

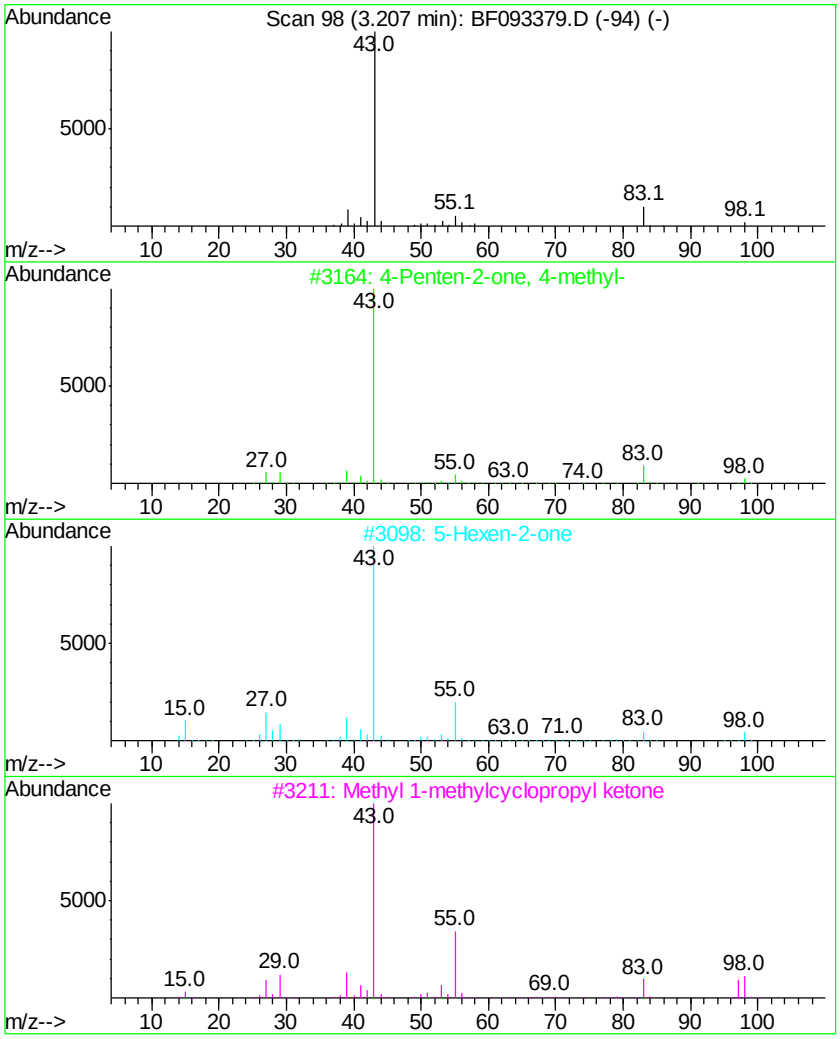
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

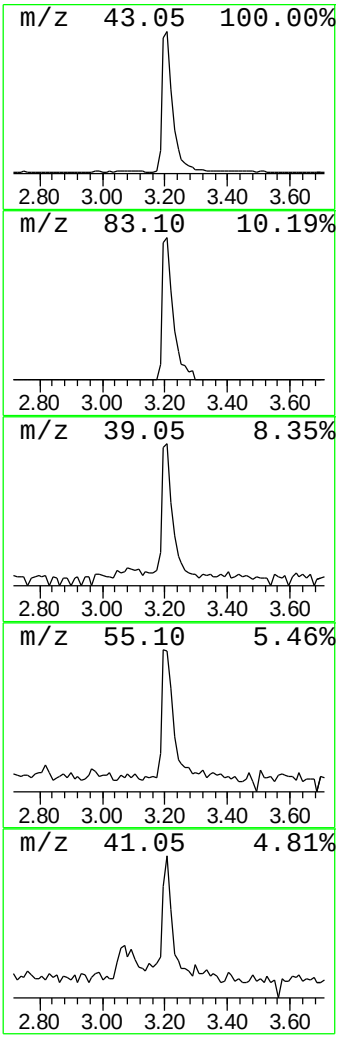
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	3.93 ng	244360	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	64
2	5-Hexen-2-one	98	C6H10O	000109-49-9	36
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	12
4	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093379.D
Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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

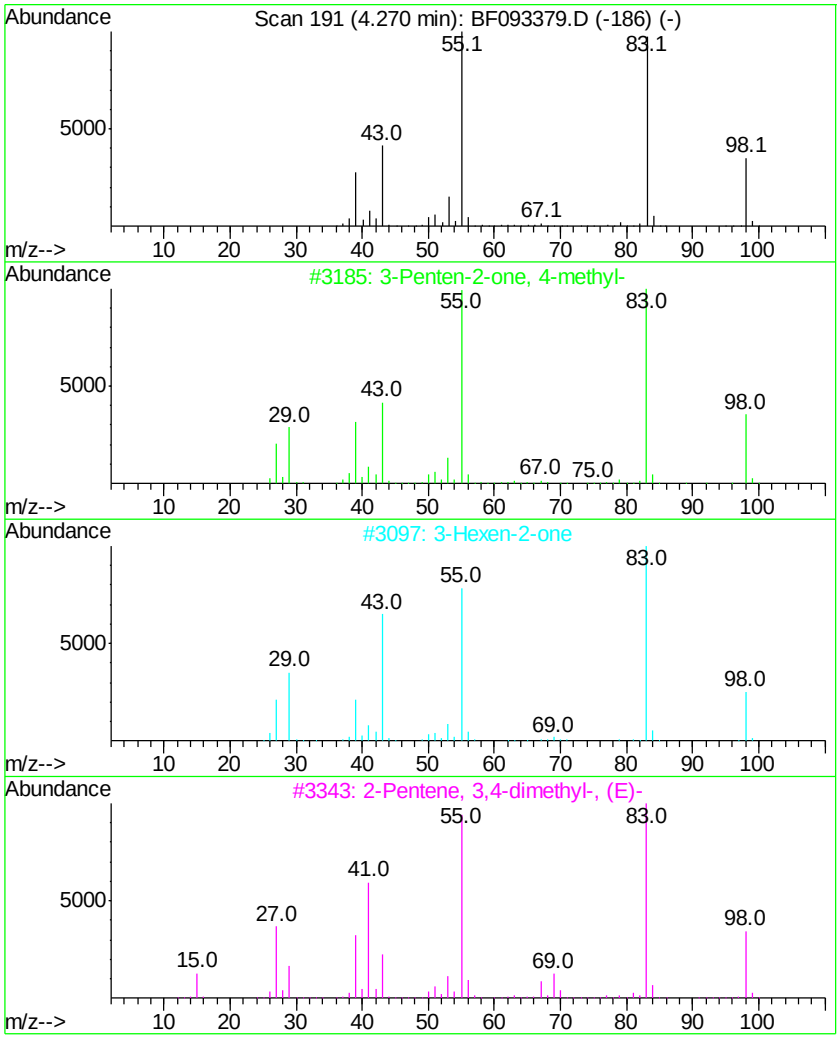
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

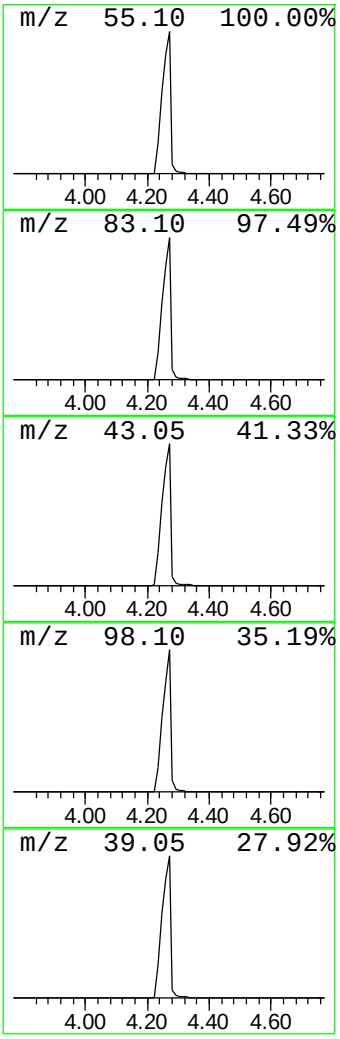
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	146.81 ng	9128240	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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093379.D
Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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

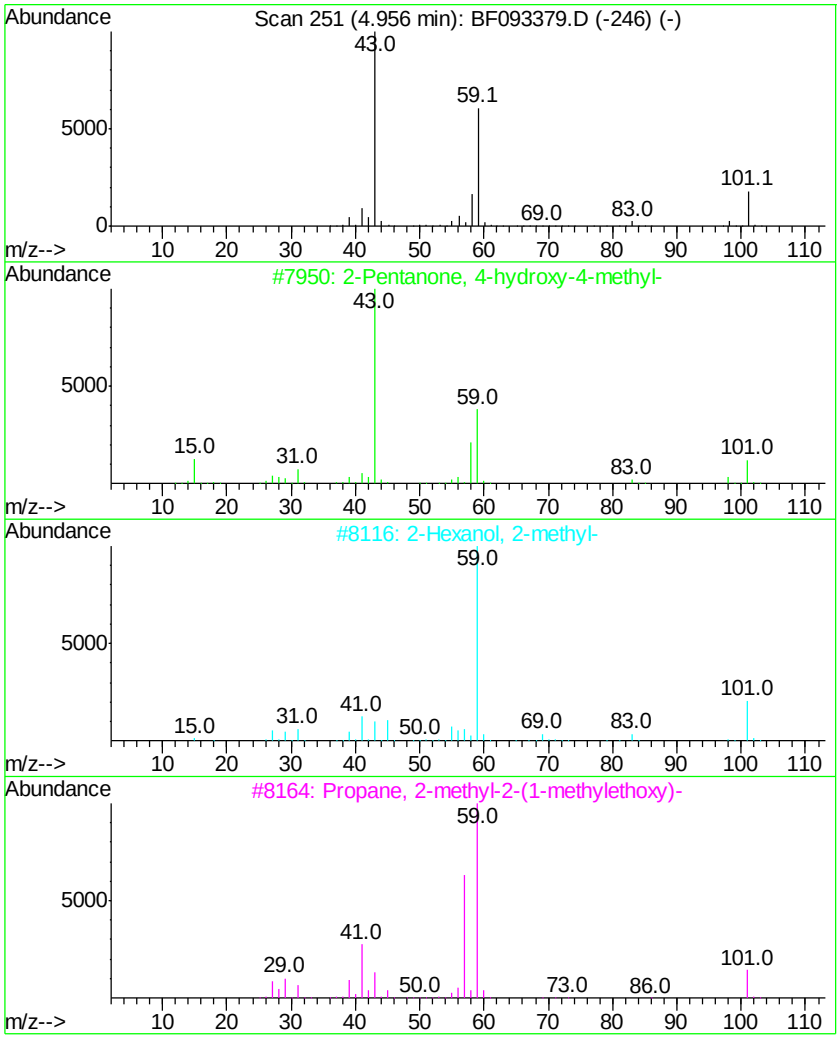
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

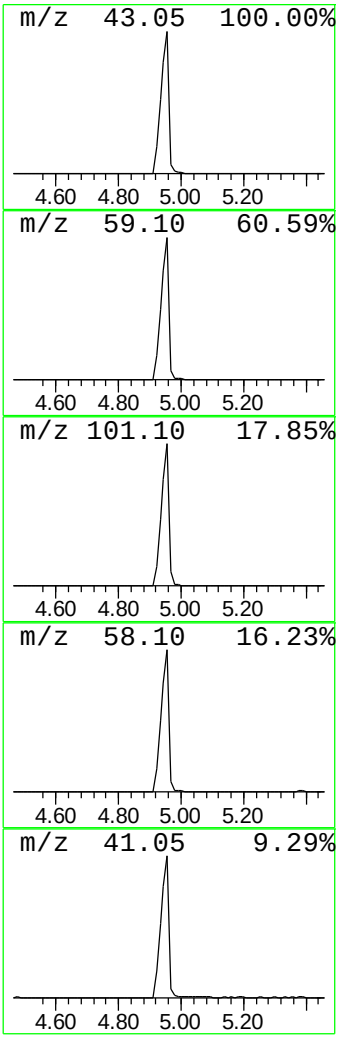
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	105.90 ng	6584400	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	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
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Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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

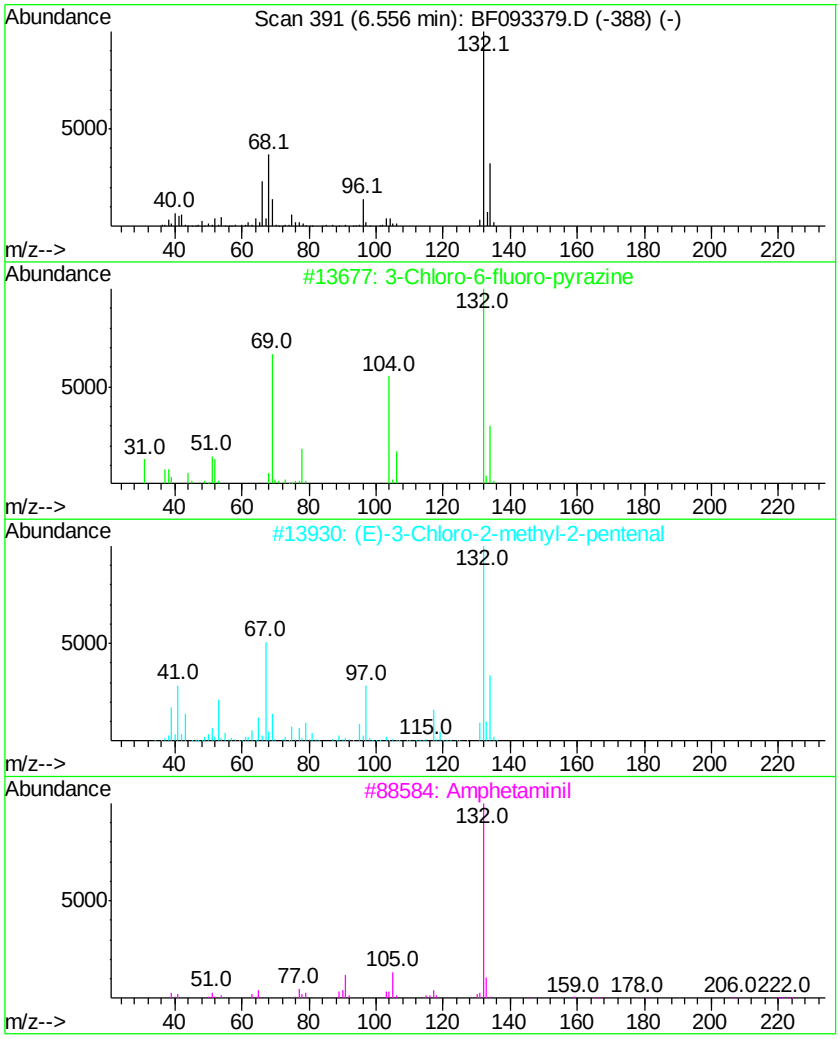
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

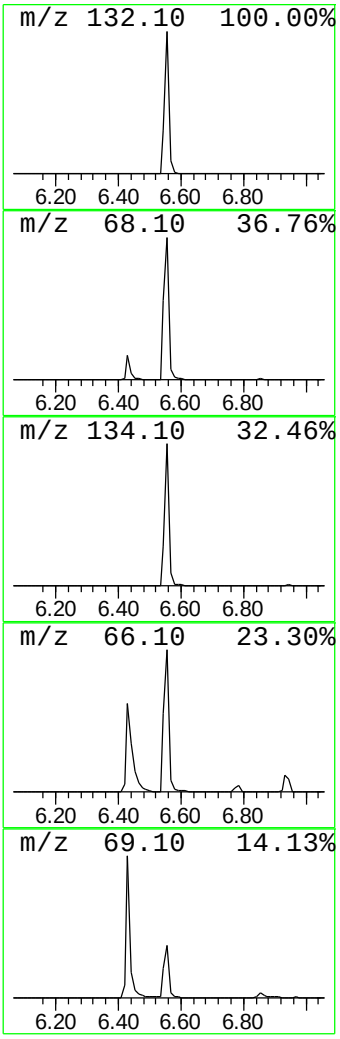
****

Peak Number 4 unknown6.56 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	15.04 ng	934949	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





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Data File : BF093379.D
Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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

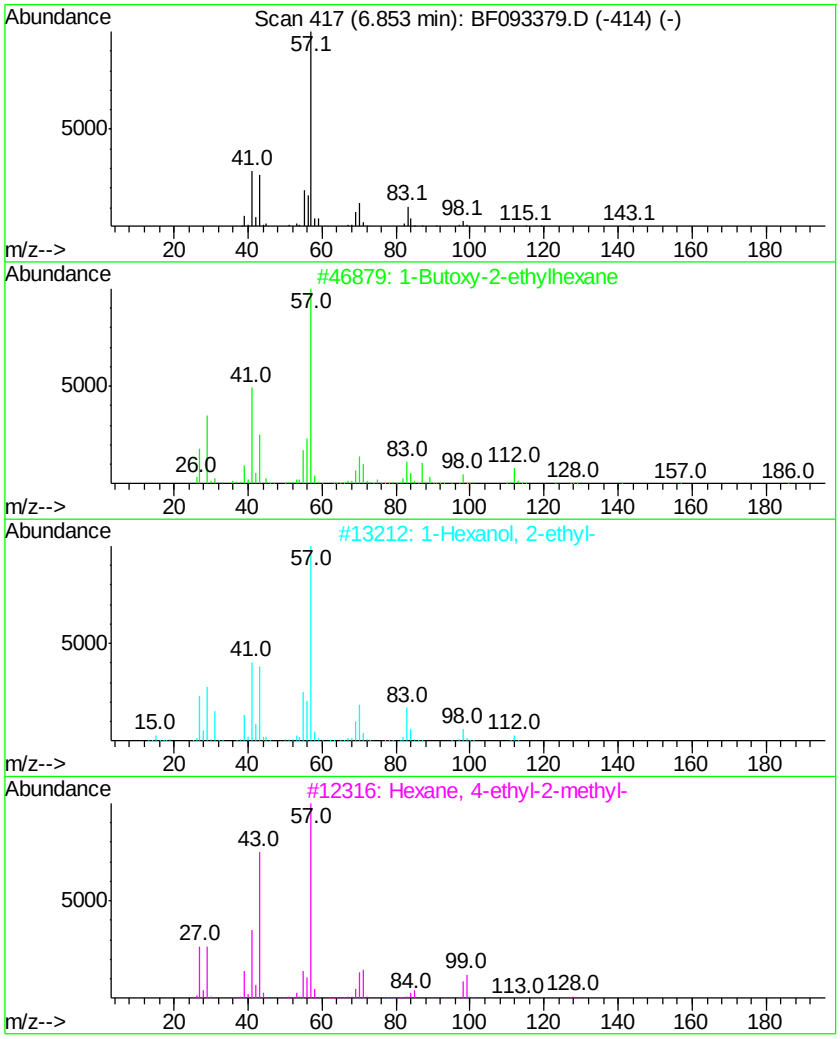
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

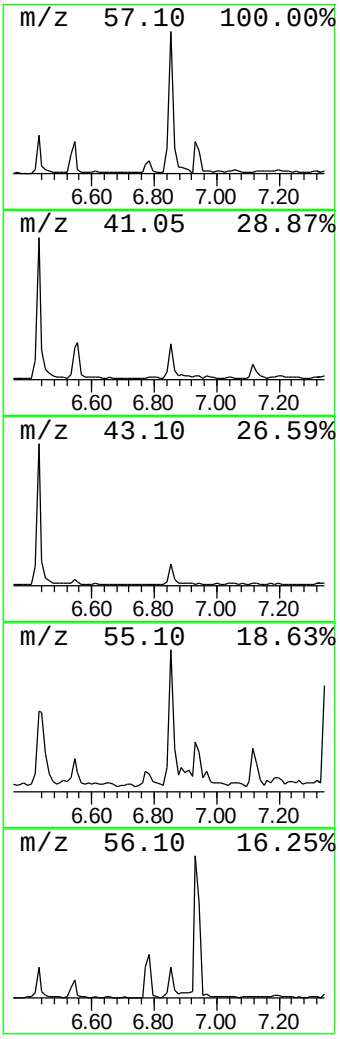
****

Peak Number 5 1-Butoxy-2-ethylhexane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.85	2.11 ng	130888	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butoxy-2-ethylhexane	186	C12H26O	062625-25-6	64
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
3	Hexane, 4-ethyl-2-methyl-	128	C9H20	003074-75-7	53
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	47





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Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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

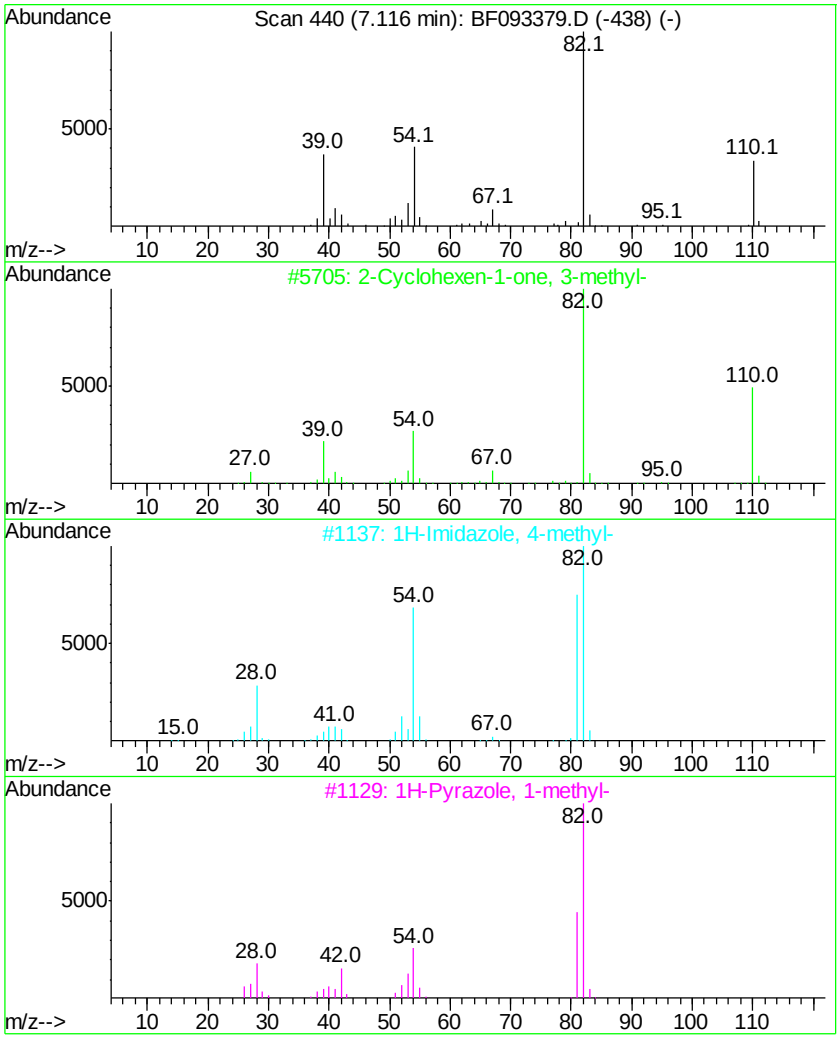
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

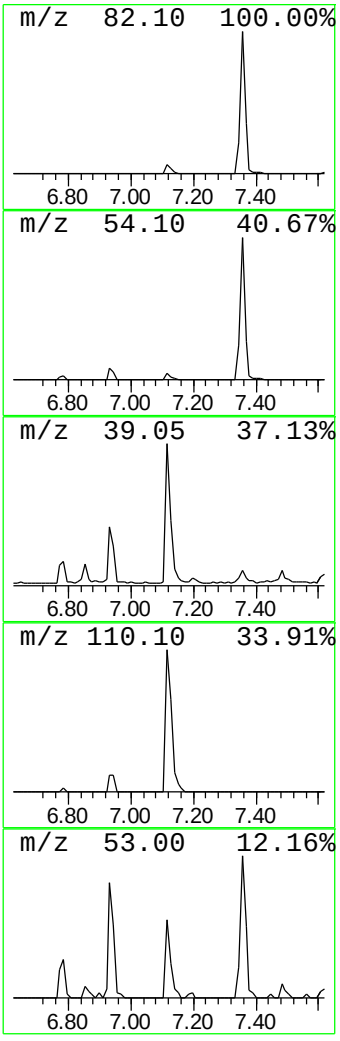
****

Peak Number 7 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	3.41 ng	212110	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	1H-Imidazole, 4-methyl-	82	C4H6N2	000822-36-6	59
3	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	47
4	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	40
5	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	39





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093379.D
Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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

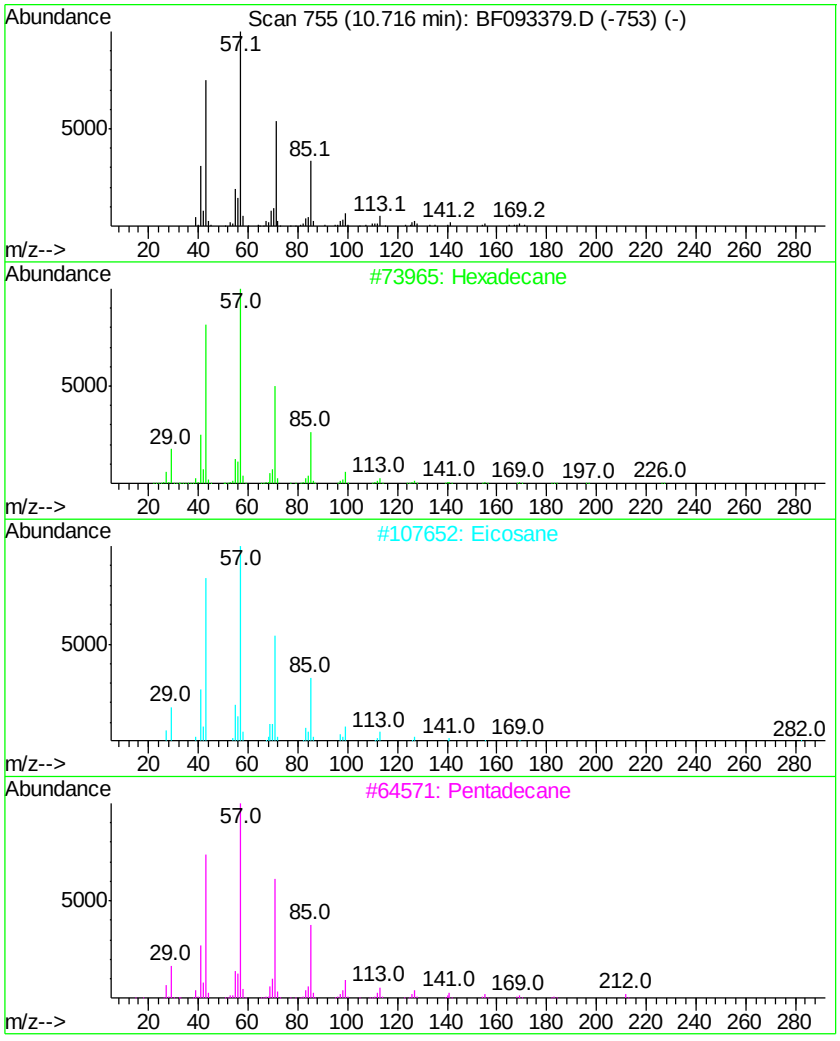
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

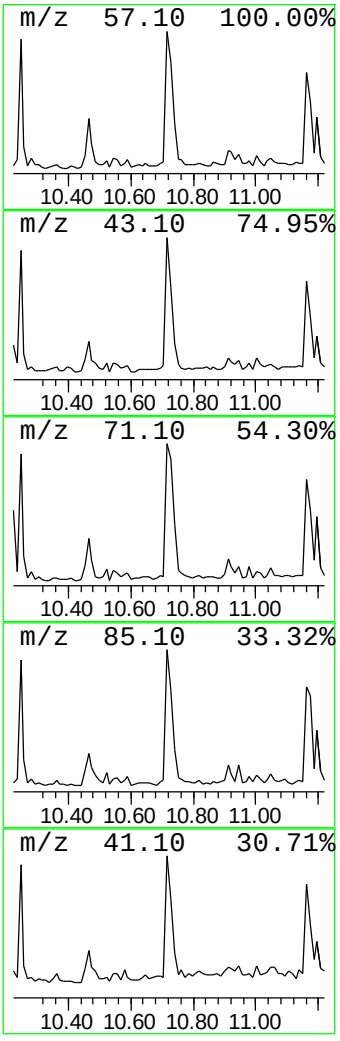
****

Peak Number 8 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	3.49 ng	319022	Phenanthrene-d10	11.30

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	Pentadecane	212	C15H32	000629-62-9	90
4	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	80
5	Tridecane	184	C13H28	000629-50-5	72





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Misc :
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Instrument : BNA_F
ClientSampleId : C-2

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

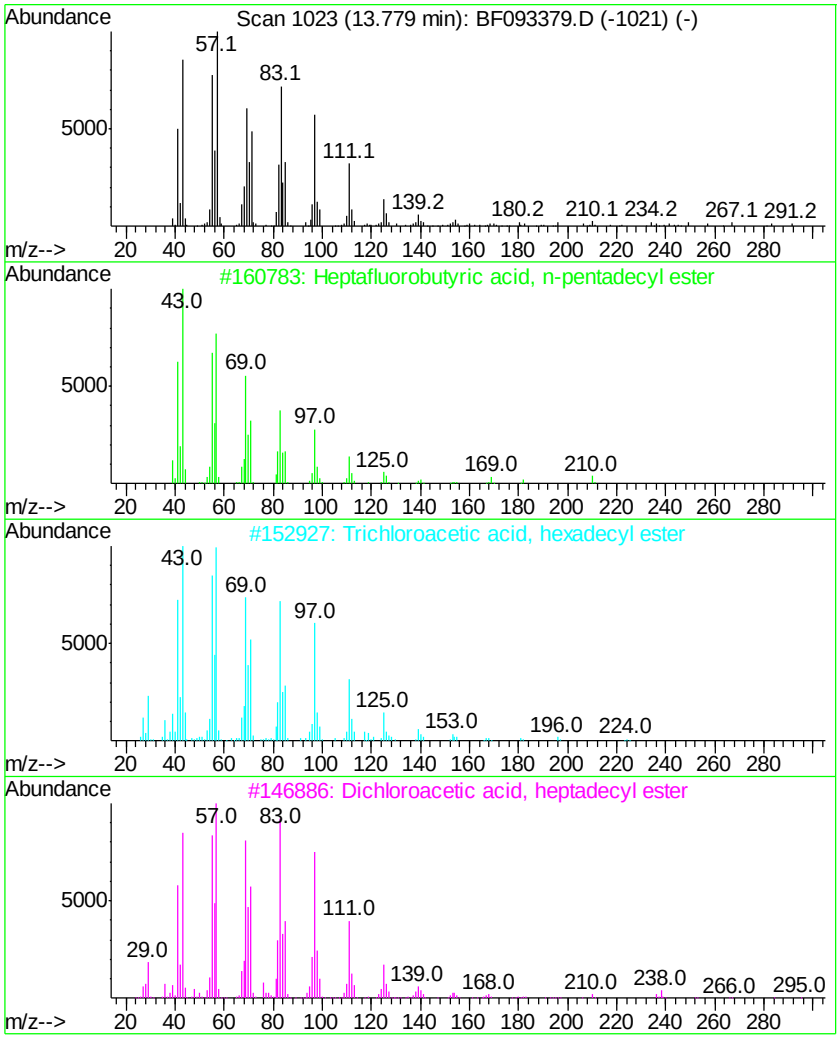
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

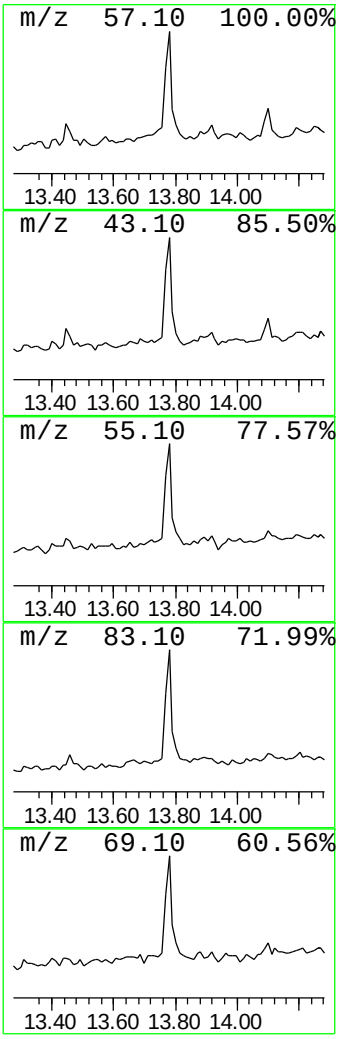
****

Peak Number 10 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	5.94 ng	376654	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90
5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093379.D
Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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

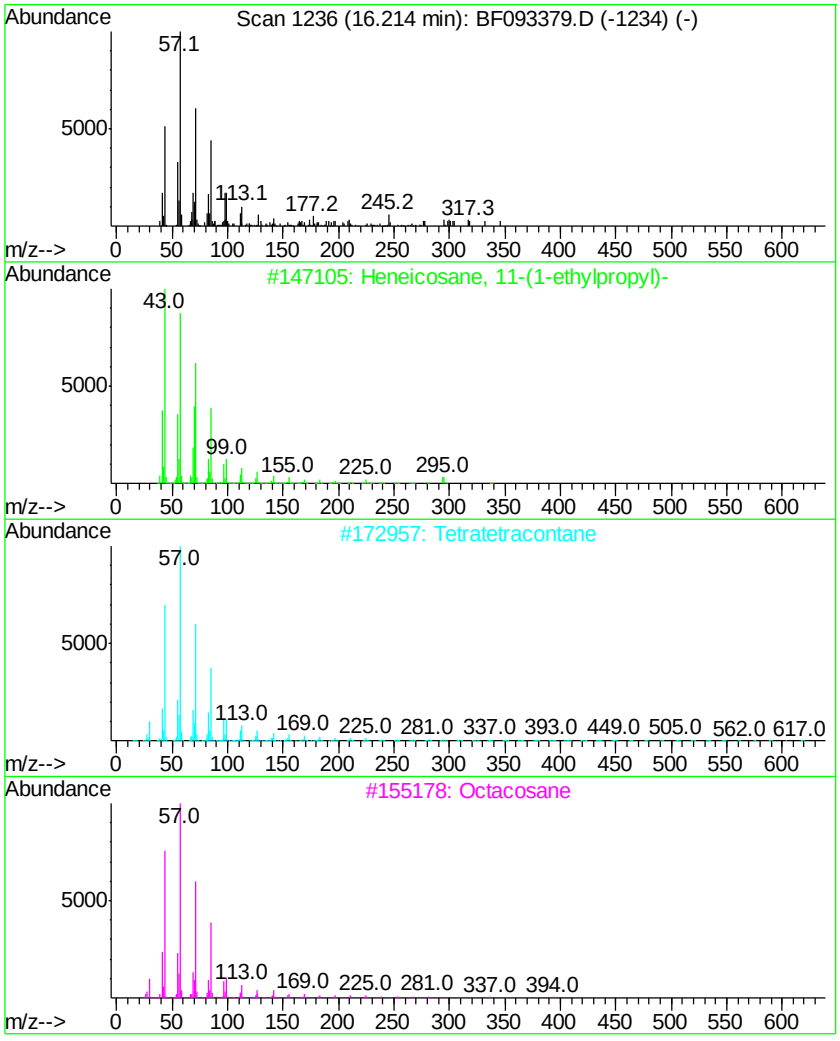
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

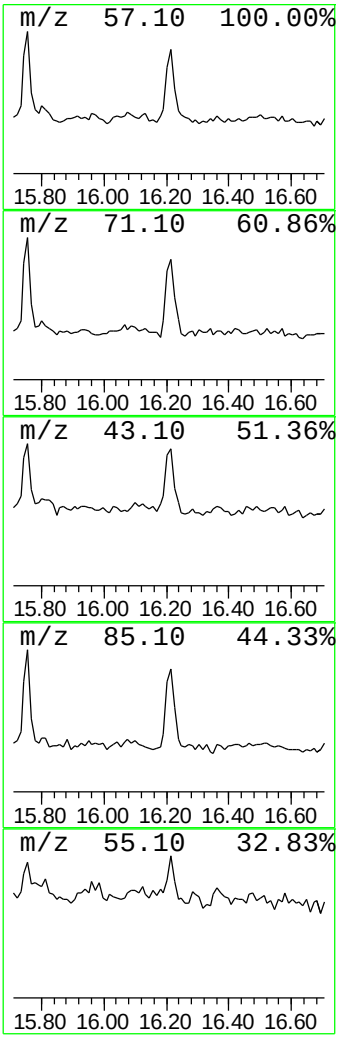
****

Peak Number 11 Heneicosane, 11-(1-ethylpro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	2.48 ng	144709	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Octadecane	254	C18H38	000593-45-3	80
5	Heptadecane	240	C17H36	000629-78-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030317\
Data File : BF093379.D
Acq On : 4 Mar 2017 00:40
Operator : SJ/MA
Sample : I2078-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-2

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	3.9	ng	244360	1	6.78	1243530	20.0
3-Penten-2-one, 4...	4.27	146.8	ng	9128240	1	6.78	1243530	20.0
2-Pentanone, 4-hy...	4.96	105.9	ng	6584400	1	6.78	1243530	20.0
unknown6.56	6.56	15.0	ng	934949	1	6.78	1243530	20.0
1-Butoxy-2-ethylh...	6.85	2.1	ng	130888	1	6.78	1243530	20.0
2-Cyclohexen-1-on...	7.12	3.4	ng	212110	1	6.78	1243530	20.0
Hexadecane	10.72	3.5	ng	319022	4	11.30	1828880	20.0
Heptafluorobutyri...	13.78	5.9	ng	376654	5	13.94	1268090	20.0
Heneicosane, 11-(...	16.21	2.5	ng	144709	6	15.36	1169160	20.0