LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093920.D
Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

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-BF032217.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	2.940	175	179	186	rVB	150811	168749	2.86%	0.375%
2	3.587	282	289	292	rVB	4407460	5890785	100.00%	13.097%
3	4.122	371	380	383	rBV	3022215	4811468	81.68%	10.697%
4	4.492	438	443	446	rBV	2221295	1995873	33.88%	4.437%
5	5.557	617	624	627	rBV	3145504	3641235	61.81%	8.095%
6	5.704	643	649	652	rBV	2740286	2917773	49.53%	6.487%
7	5.957	688	692	696	rBV	1148285	1009406	17.14%	2.244%
8	6.139	718	723	726	rVB	3352638	3327072	56.48%	7.397%
9	6.322	750	754	757	rBV	251890	221946	3.77%	0.493%
10	6.604	796	802	805	rBV	2290277	2768953	47.00%	6.156%
11	6.769	823	830	833	rBV2	65477	68782	1.17%	0.153%
12	6.892	847	851	859	rBV3	74925	115344	1.96%	0.256%
13	7.463	942	948	952	rBV	1395988	1406149	23.87%	3.126%
14	8.786	1166	1173	1176	rBV	4444902	4977765	84.50%	11.067%
15	9.280	1251	1257	1261	rBV	247531	245770	4.17%	0.546%
16	9.498	1283	1294	1303	rBV4	93825	226339	3.84%	0.503%
17	9.604	1308	1312	1316	rVB2	1511254	1542443	26.18%	3.429%
18	9.933	1363	1368	1371	rBV3	51720	94889	1.61%	0.211%
19	10.192	1408	1412	1416	rVB	126122	111608	1.89%	0.248%
20	10.469	1452	1459	1462	rBV	45541	71643	1.22%	0.159%
21	10.568	1472	1476	1479	rBV	437193	404548	6.87%	0.899%
22	10.698	1494	1498	1503	rVB	91257	91151	1.55%	0.203%
23	10.774	1508	1511	1514	rBV	124873	150433	2.55%	0.334%
24	11.233	1584	1589	1592	rBV	138164	155282	2.64%	0.345%
25	11.333	1602	1606	1609	rBV	89297	86357	1.47%	0.192%
26	11.427	1617	1622	1625	rVV	1483110	1494104	25.36%	3.322%
27	12.927	1874	1877	1880	rVB	79481	71513	1.21%	0.159%
28	13.192	1918	1922	1925	rBV	75968	79489	1.35%	0.177%
29	13.409	1952	1959	1963	rBV2	3516147	4332797	73.55%	9.633%
30	14.556	2151	2154	2165	rBV	262681	320429	5.44%	0.712%
31	14.680	2169	2175	2178	rBV	1111444	1270779	21.57%	2.825%
32	16.315	2447	2453	2462	rBV	718892	908296	15.42%	2.019%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093920.D
Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

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-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 44979170

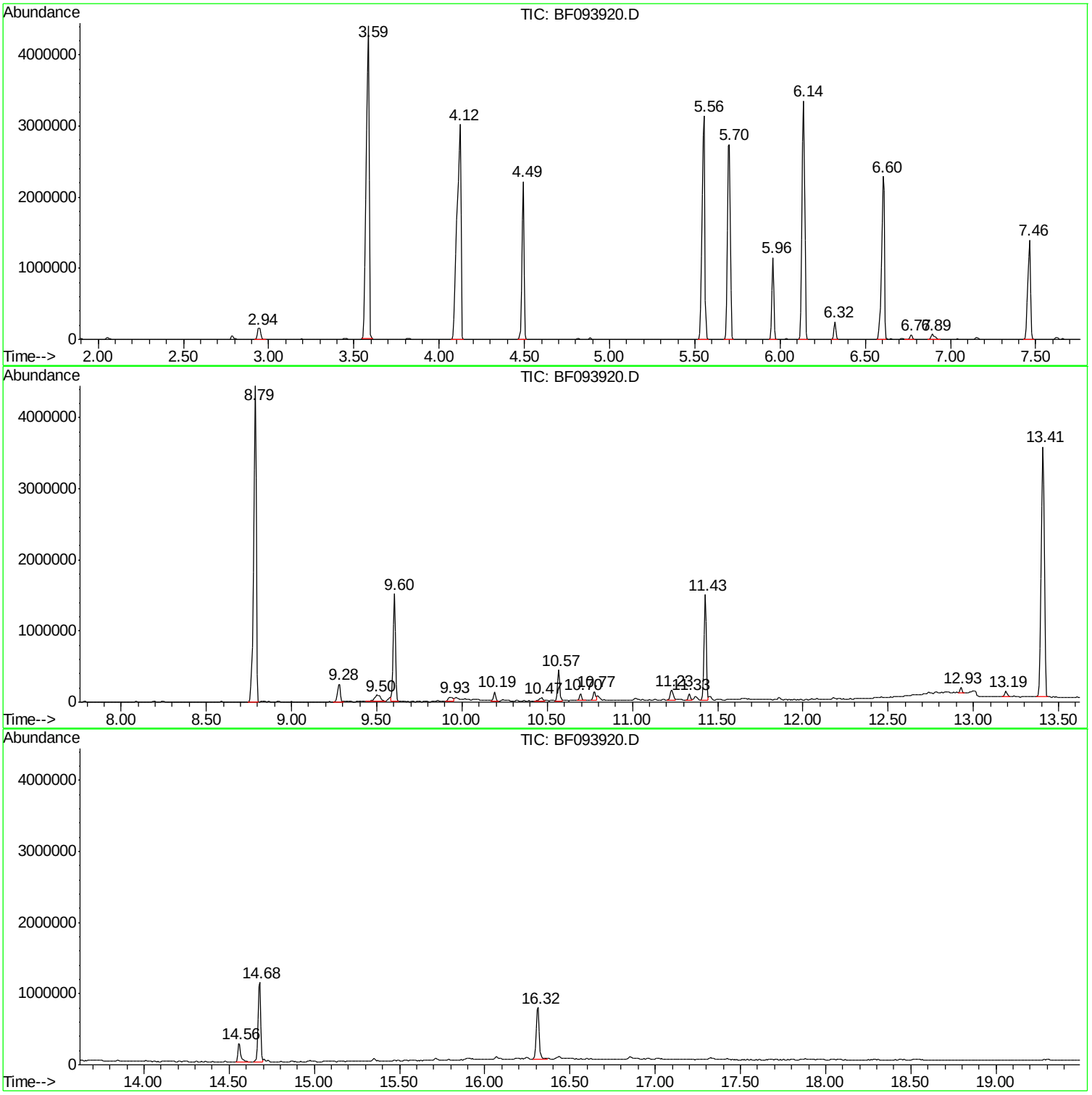
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093920.D
Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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Data File : BF093920.D
Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

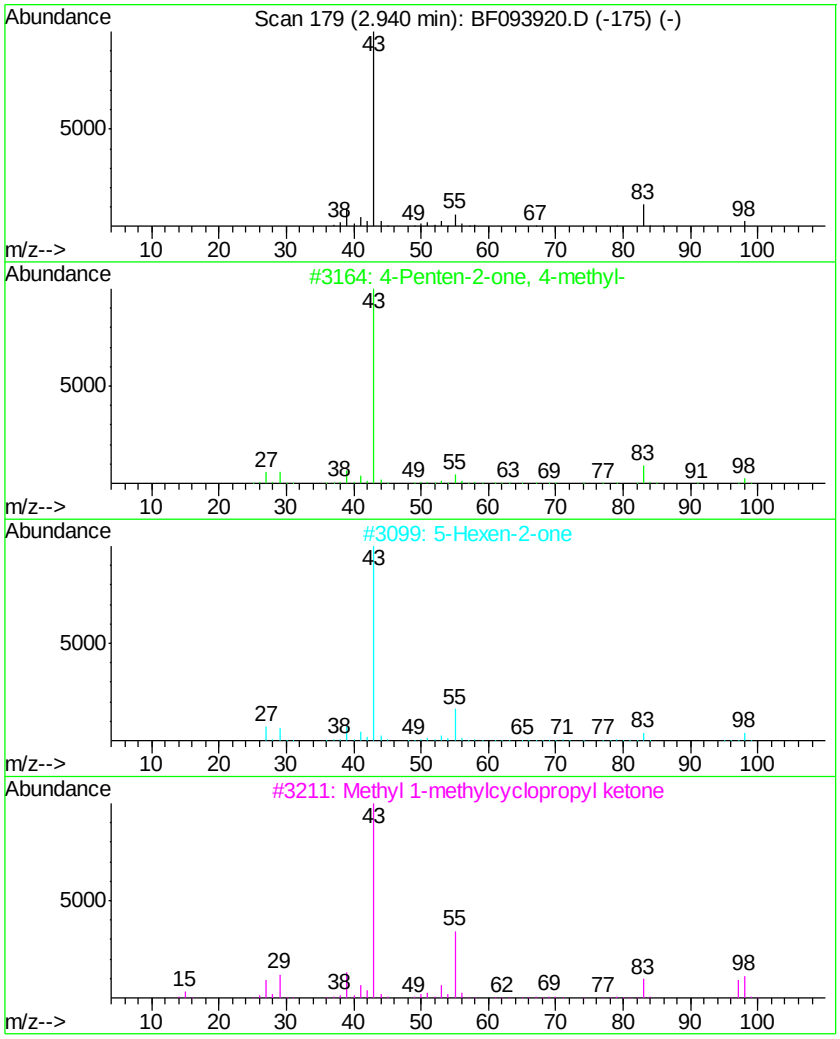
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

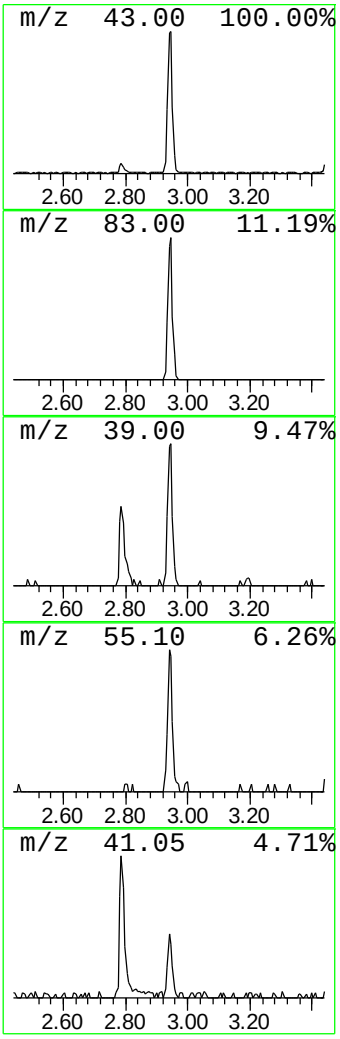
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.94	3.34 ng	168749	1,4-Dichlorobenzene-d4	5.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	5-Hexen-2-one	98	C6H10O	000109-49-9	46
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	43
4	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	23
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093920.D
Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

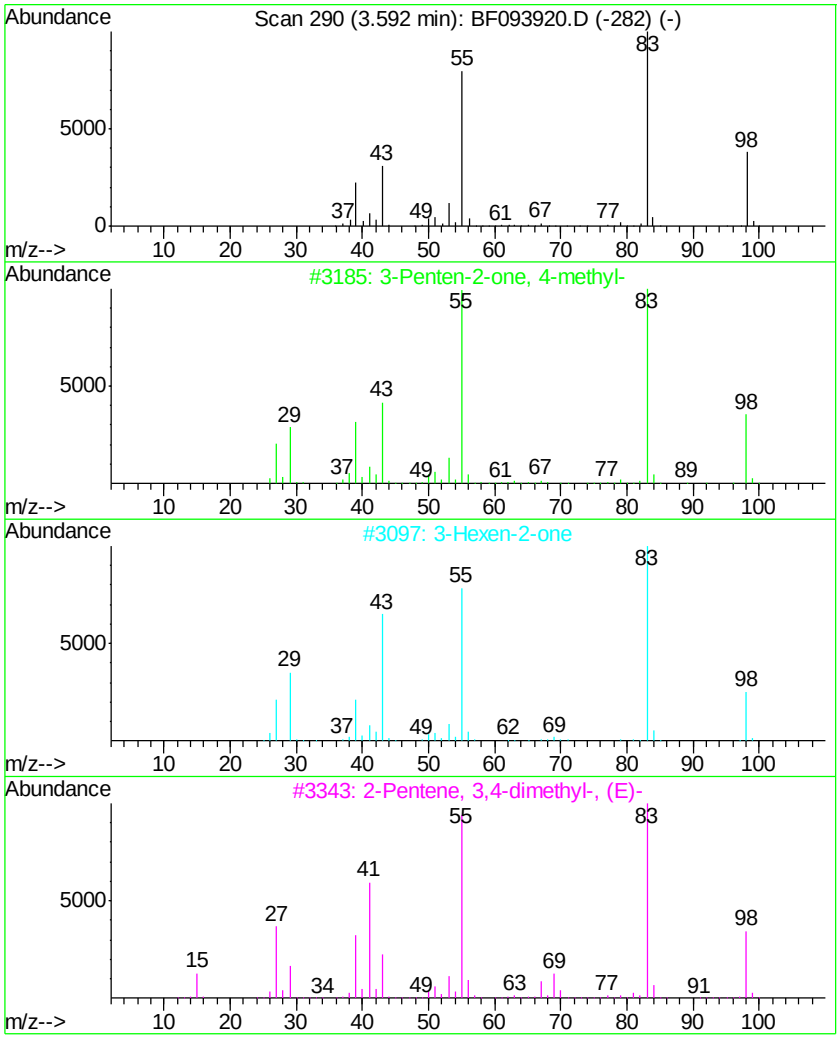
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

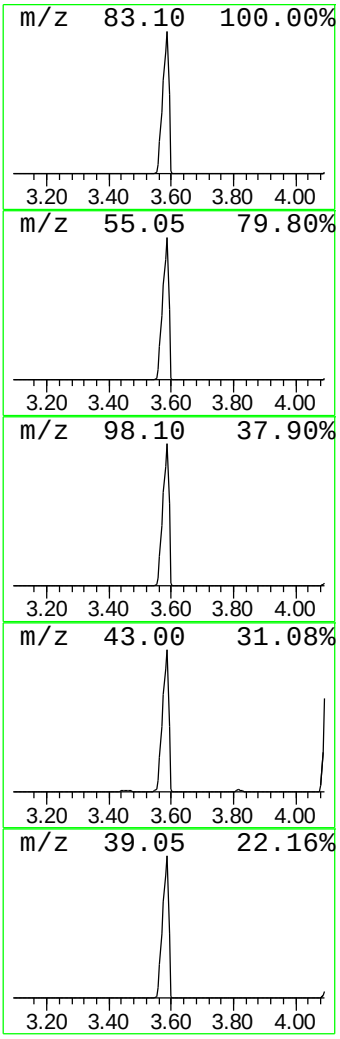
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	116.72 ng	5890790	1,4-Dichlorobenzene-d4	5.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
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	80





Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093920.D
Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

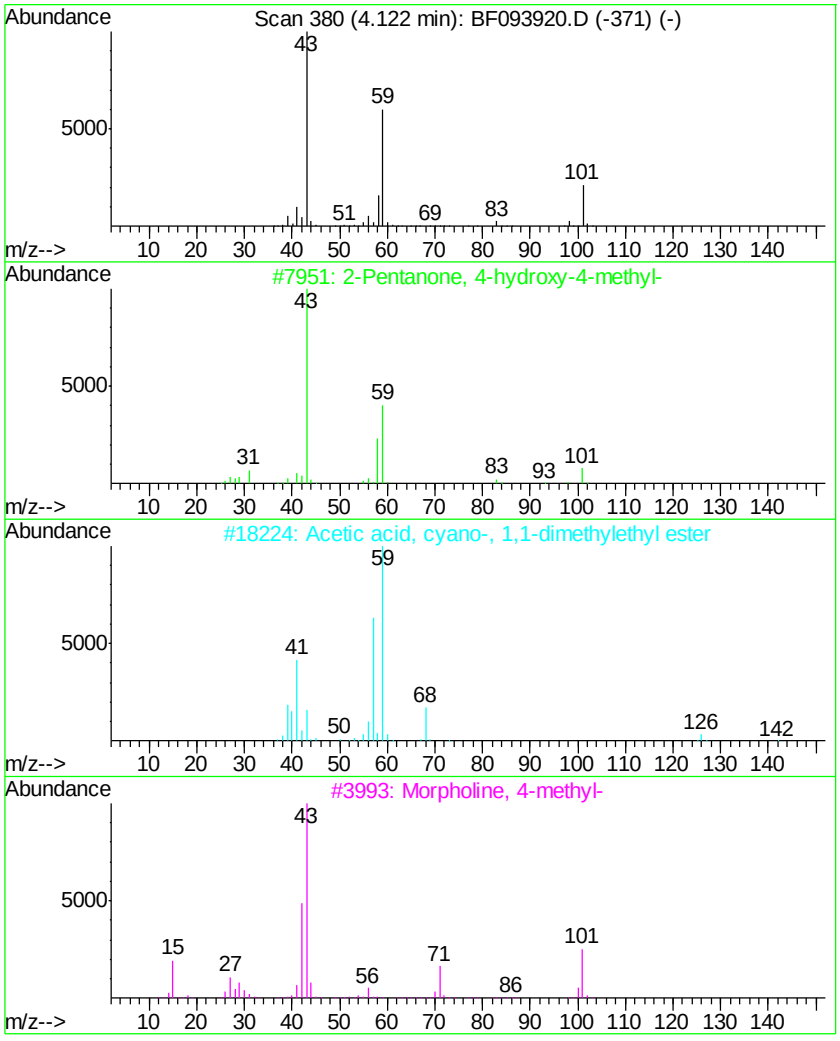
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

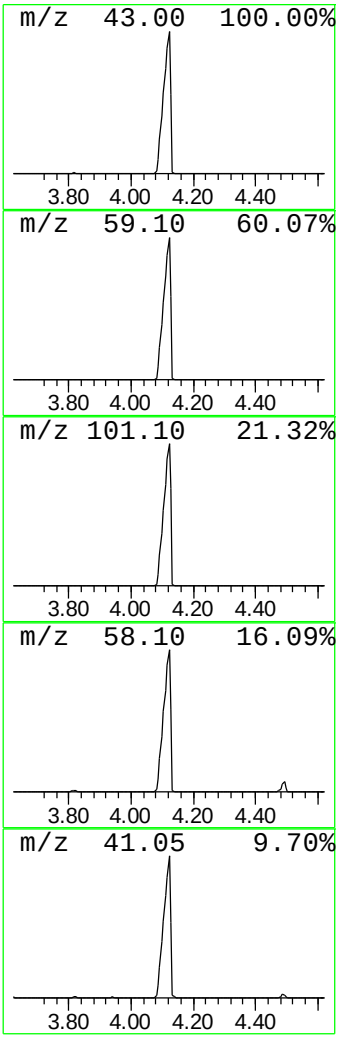
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.12	95.33 ng	4811470	1,4-Dichlorobenzene-d4	5.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9





Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093920.D
Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

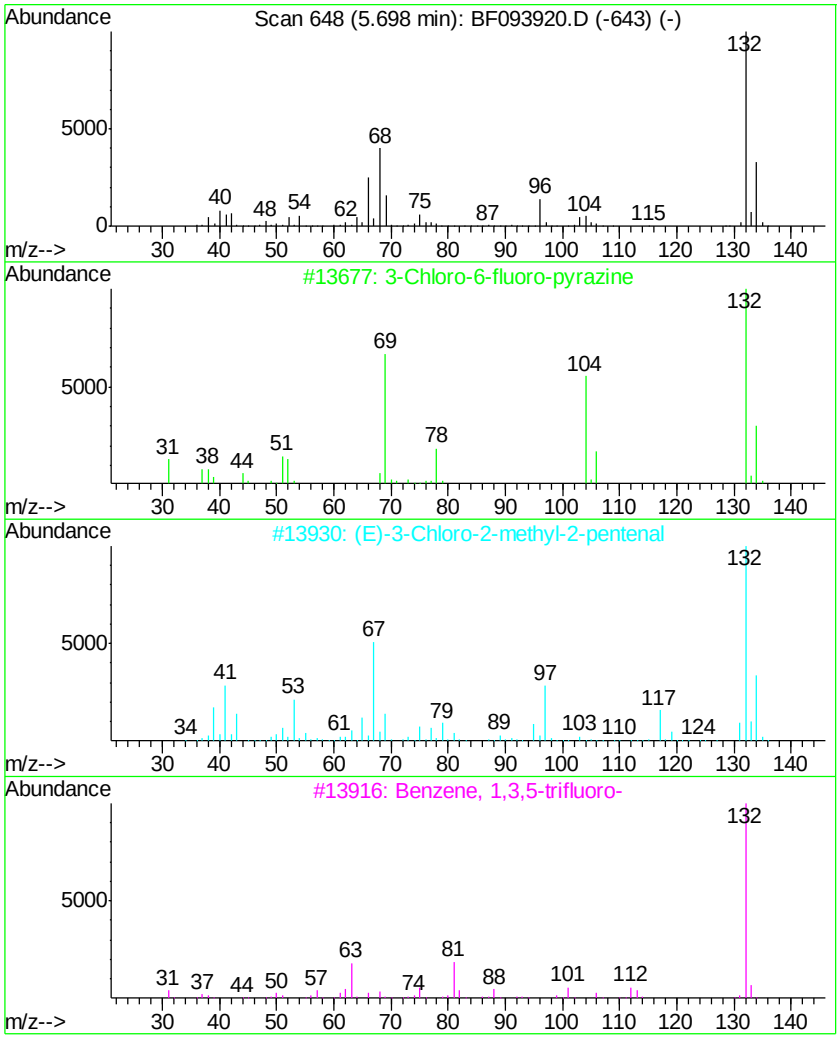
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

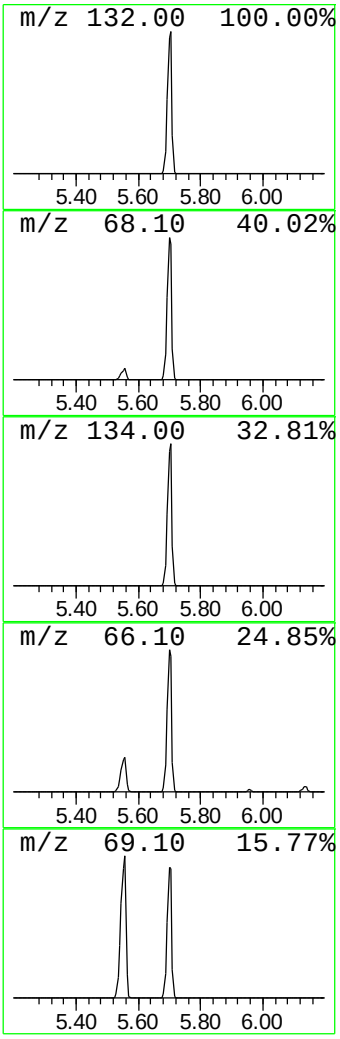
****

Peak Number 4 unknown5.70 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	57.81 ng	2917770	1,4-Dichlorobenzene-d4	5.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093920.D
Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

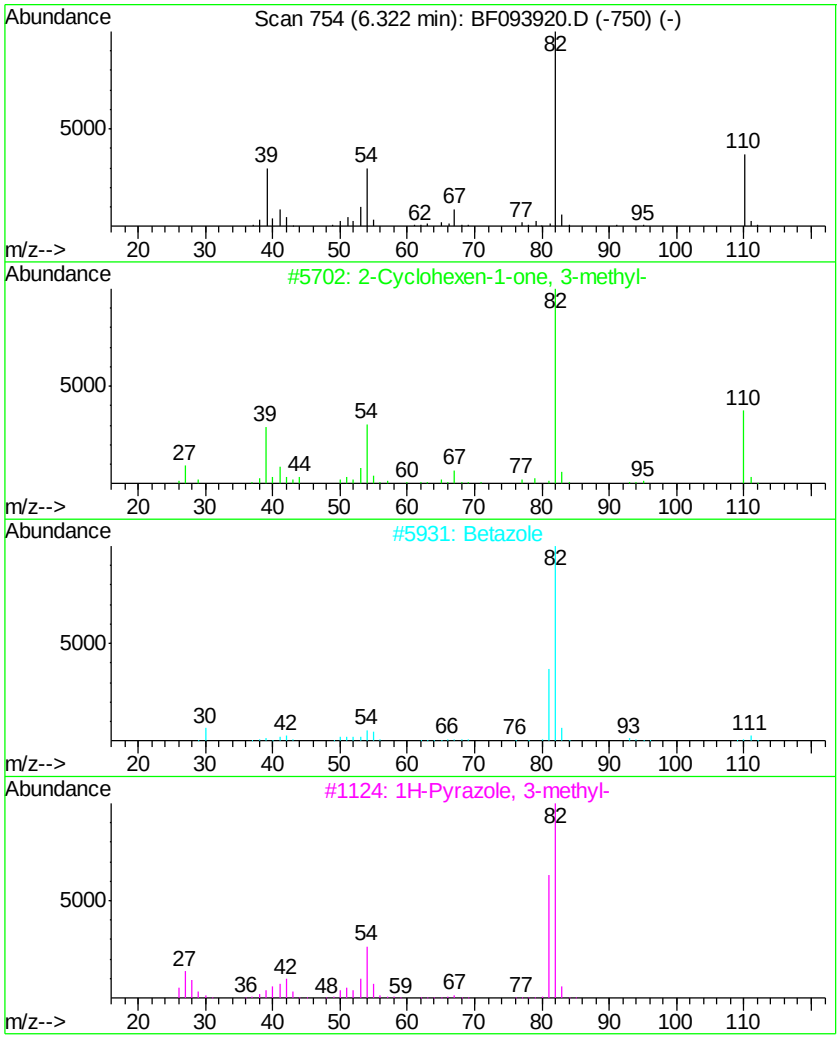
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

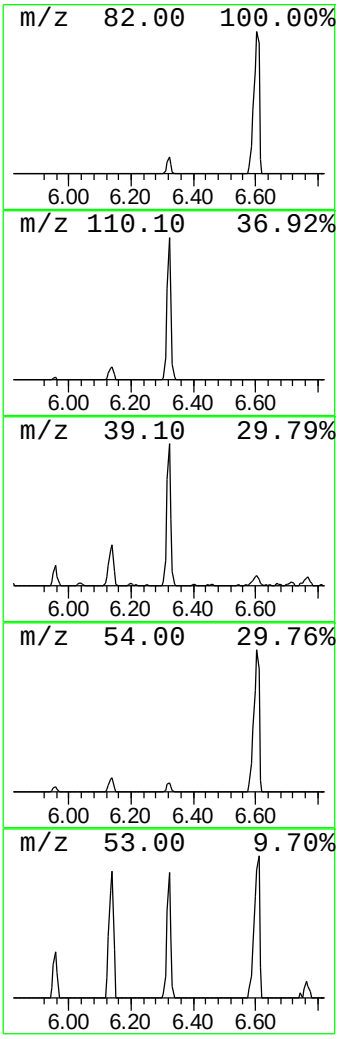
****

Peak Number 6 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	4.40 ng	221946	1,4-Dichlorobenzene-d4	5.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	Betazole	111	C5H9N3	000105-20-4	50
3	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	50
4	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	45
5	1H-Imidazole, 4-methyl-	82	C4H6N2	000822-36-6	42





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Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

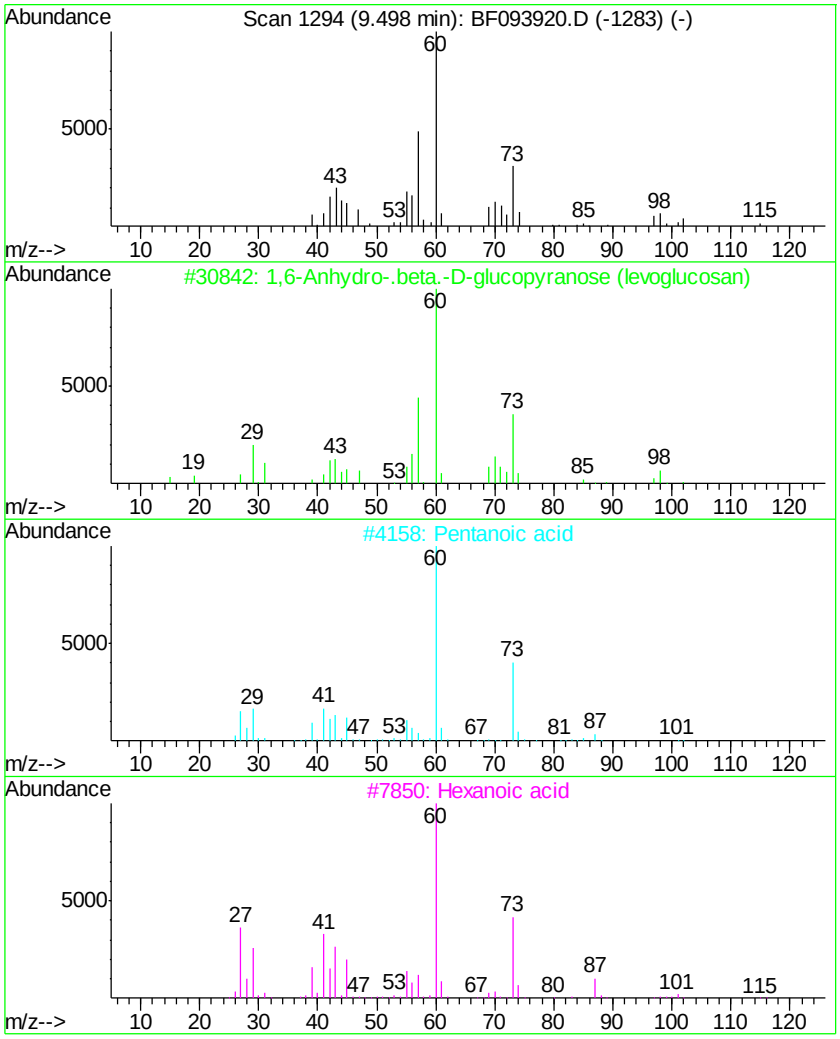
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

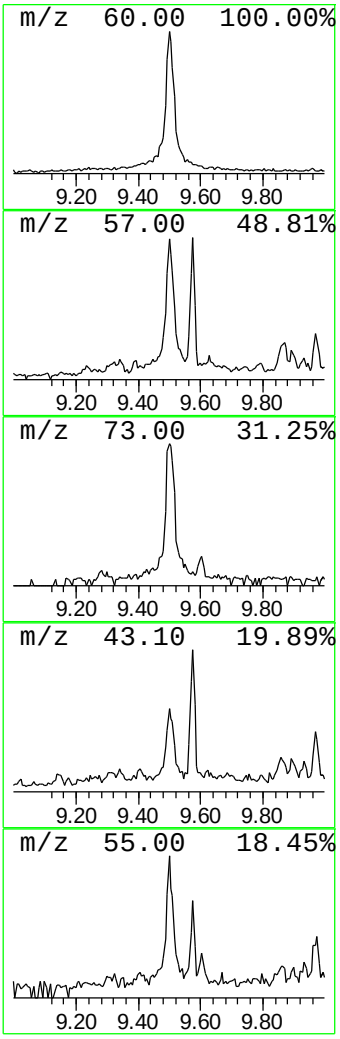
****

Peak Number 7 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	2.93 ng	226339	Acenaphthene-d10	9.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	72
2	Pentanoic acid	102	C5H10O2	000109-52-4	50
3	Hexanoic acid	116	C6H12O2	000142-62-1	50
4	Heptanoic acid	130	C7H14O2	000111-14-8	50
5	L-Mannose, 6-deoxy-	164	C6H12O5	003615-41-6	45





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Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

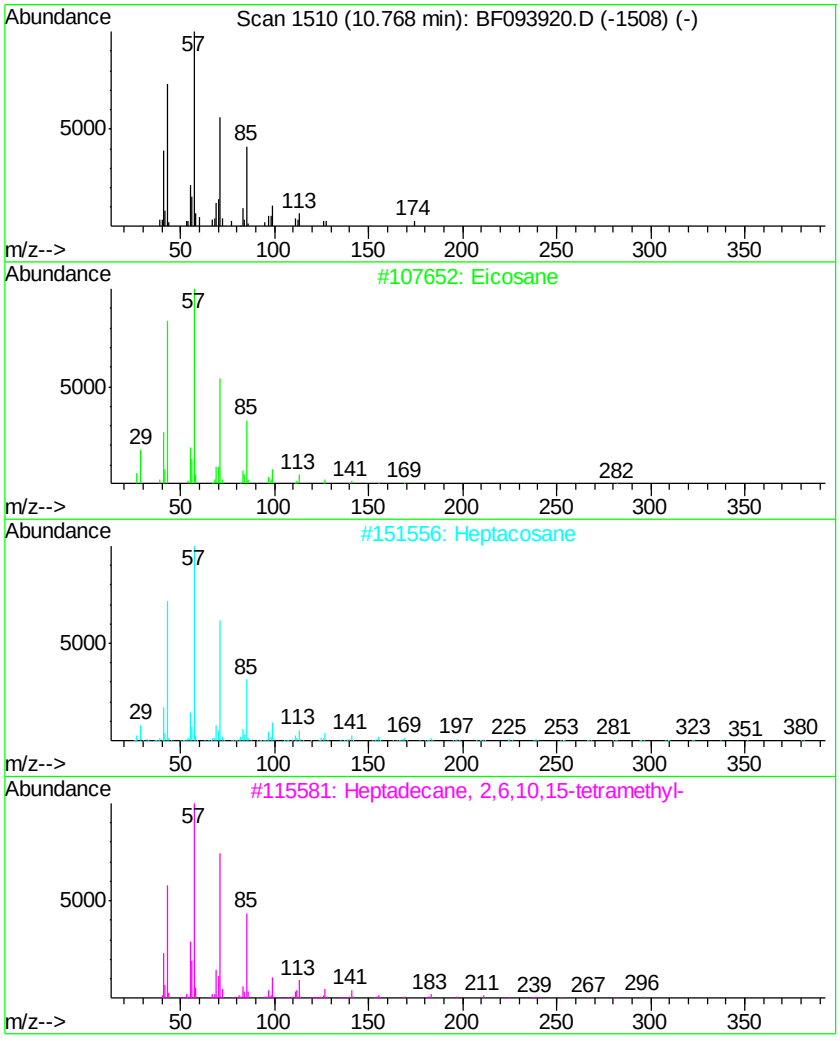
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

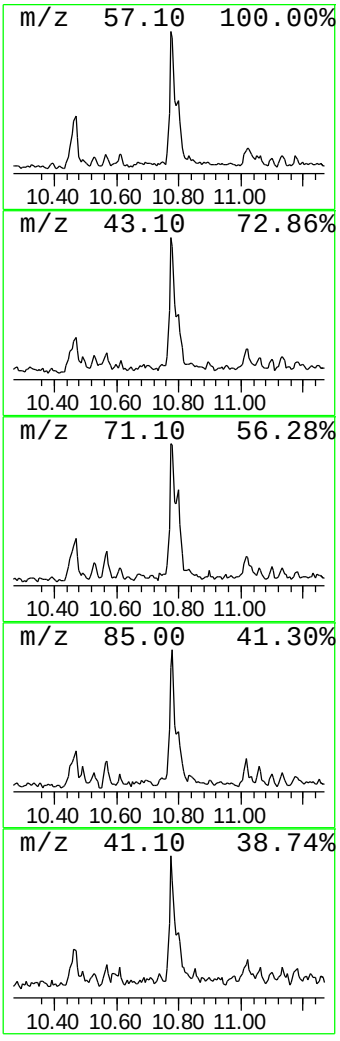
****

Peak Number 8 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.01 ng	150433	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4	Hexadecane	226	C16H34	000544-76-3	86
5	Tetracosane	338	C24H50	000646-31-1	86





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Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

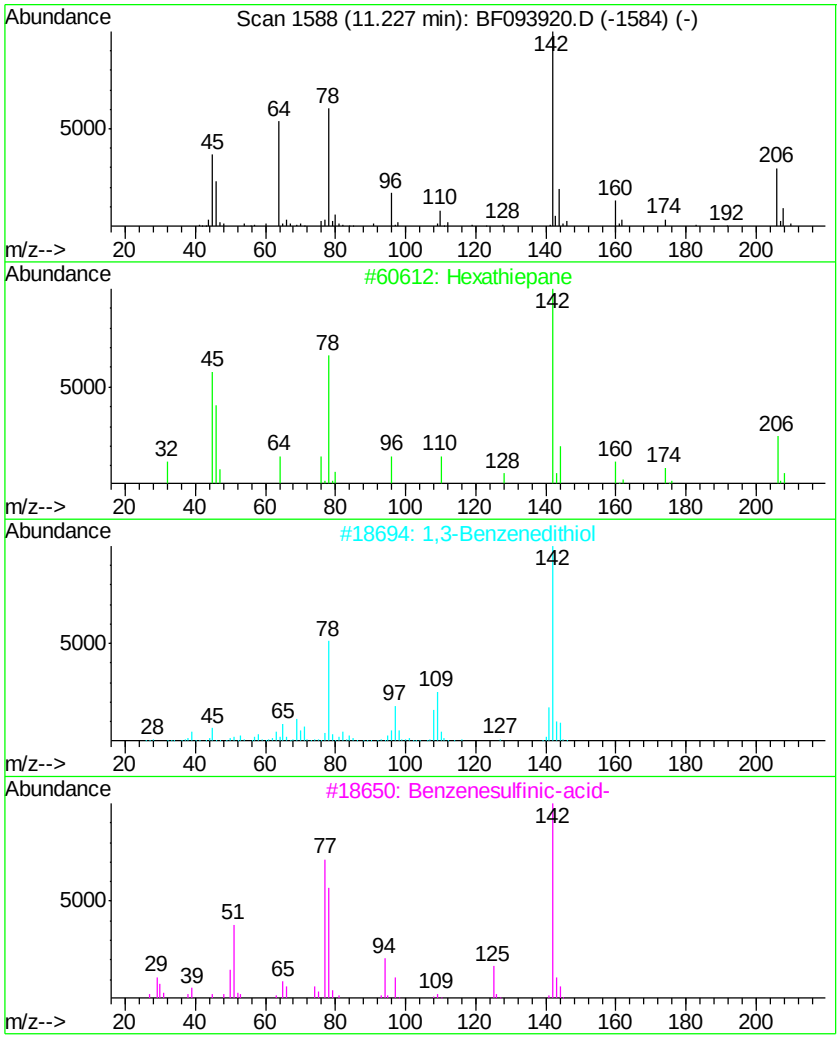
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

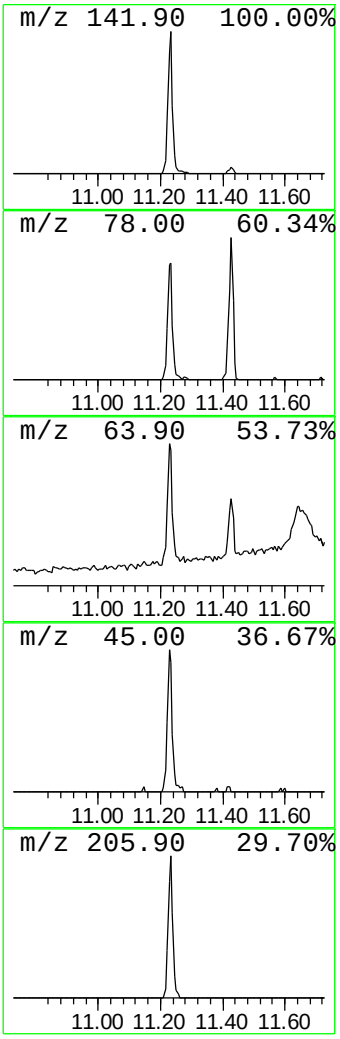
****

Peak Number 9 Hexathiepane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.23	2.08 ng	155282	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiepane	206	CH2S6	017233-71-5	55
2	1,3-Benzenedithiol	142	C6H6S2	000626-04-0	9
3	Benzenesulfinic-acid-	142	C6H6O2S	000618-41-7	9
4	Phosphinic acid, (1,1-dimethylet...	198	C10H15O2P	004923-86-8	9
5	Dibutyl(3-nonyn-1-yl)amine	251	C17H33N	063791-59-3	9





Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093920.D
Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

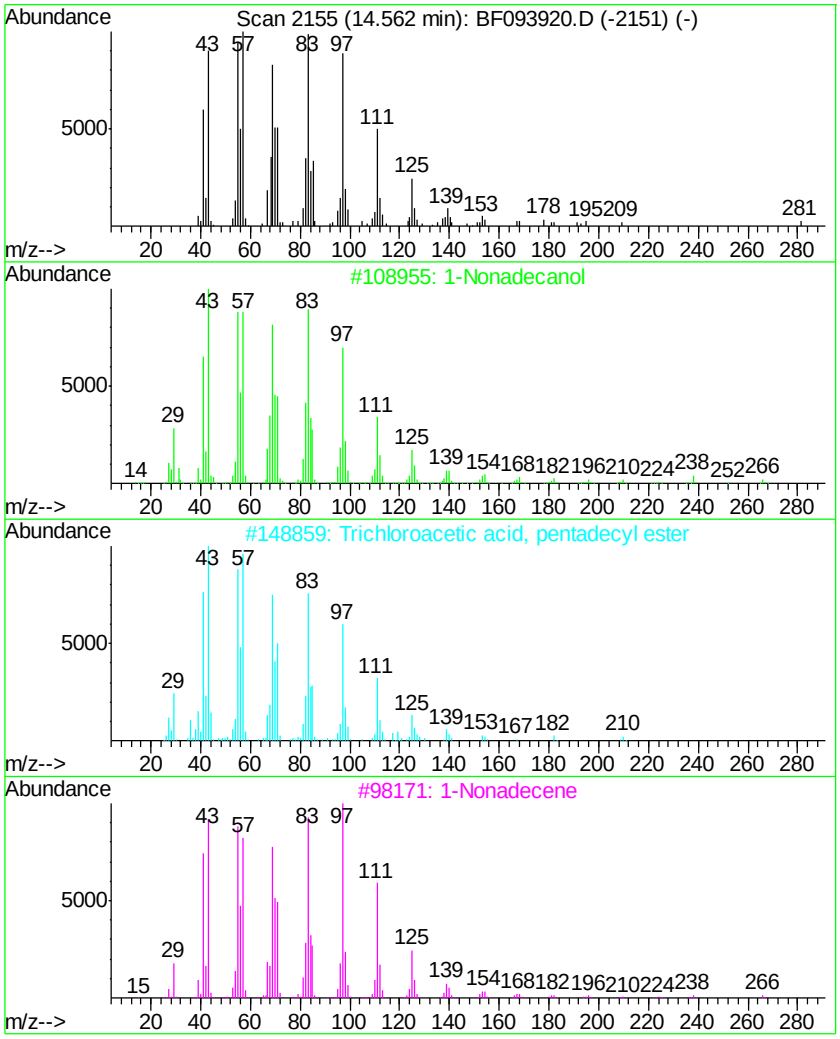
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

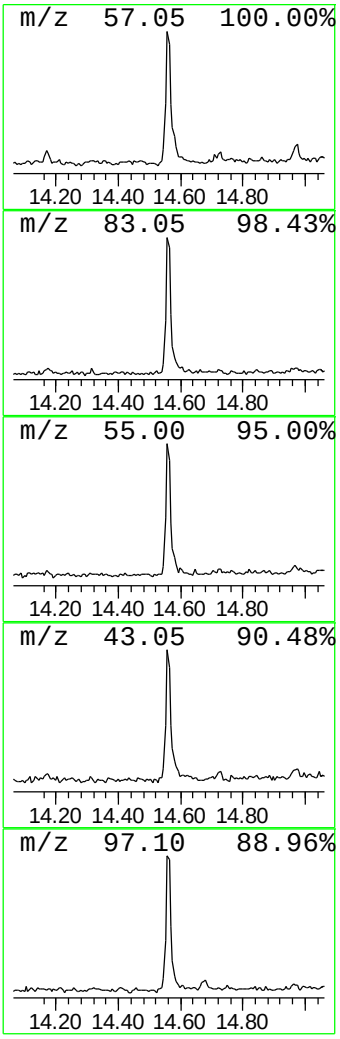
****

Peak Number 10 1-Nonadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	5.04 ng	320429	Chrysene-d12	14.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecanol	284	C19H40O	001454-84-8	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\Data\BF032417\
Data File : BF093920.D
Acq On : 24 Mar 2017 21:36
Operator : SJ/MA
Sample : I2381-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-1-2-DENSEGRADEAGGREGATE-

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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...	2.94	3.3	ng	168749	1	5.96	1009410	20.0
3-Penten-2-one, 4...	3.59	116.7	ng	5890790	1	5.96	1009410	20.0
2-Pentanone, 4-hy...	4.12	95.3	ng	4811470	1	5.96	1009410	20.0
unknown5.70	5.70	57.8	ng	2917770	1	5.96	1009410	20.0
2-Cyclohexen-1-on...	6.32	4.4	ng	221946	1	5.96	1009410	20.0
1,6-Anhydro-.beta...	9.50	2.9	ng	226339	3	9.60	1542440	20.0
Eicosane	10.77	2.0	ng	150433	4	11.43	1494100	20.0
Hexathiepane	11.23	2.1	ng	155282	4	11.43	1494100	20.0
1-Nonadecanol	14.56	5.0	ng	320429	5	14.68	1270780	20.0