LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

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-BF123115.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	4.339	194	197	201	rBV	365060	492019	5.40%	0.830%
2	5.002	252	255	257	rBV	2408120	2764637	30.33%	4.663%
3	5.424	290	292	295	rVB	3084597	2876413	31.55%	4.851%
4	5.824	325	327	330	rBV	440315	380474	4.17%	0.642%
5	6.316	367	370	373	rBV	152437	154226	1.69%	0.260%
6	6.453	380	382	385	rVB	1354179	1720619	18.88%	2.902%
7	6.590	391	394	396	rBV	5770113	5006462	54.92%	8.444%
8	6.819	412	414	418	rVB	2309397	2021337	22.17%	3.409%
9	6.979	425	428	430	rVB	7304059	6479558	71.08%	10.929%
10	7.390	461	464	466	rVB	5331258	5512311	60.47%	9.297%
11	7.642	483	486	492	rVB	193295	330152	3.62%	0.557%
12	8.110	524	527	529	rBV	2674861	2475313	27.15%	4.175%
13	8.670	570	576	578	rBV3	147068	308313	3.38%	0.520%
14	8.762	581	584	586	rVV	323229	373300	4.10%	0.630%
15	9.185	618	621	624	rBV	6256834	9115699	100.00%	15.375%
16	9.585	654	656	658	rBV	291645	243393	2.67%	0.411%
17	9.779	670	673	674	rBV	63051	112259	1.23%	0.189%
18	9.802	674	675	676	rVV	129124	99270	1.09%	0.167%
19	9.859	678	680	683	rVB	2049704	2406079	26.39%	4.058%
20	10.305	715	719	720	rVB2	136689	201972	2.22%	0.341%
21	10.522	734	738	739	rBV2	54938	103831	1.14%	0.175%
22	10.648	747	749	752	rBV2	3011706	3591183	39.40%	6.057%
23	10.774	758	760	764	rVB	167875	183568	2.01%	0.310%
24	11.345	808	810	812	rBV	2375240	2132219	23.39%	3.596%
25	11.894	856	858	861	rBV2	194940	245331	2.69%	0.414%
26	12.134	877	879	881	rBV	115116	113185	1.24%	0.191%
27	12.934	947	949	952	rBV	4859955	6274907	68.84%	10.584%
28	13.848	1027	1029	1033	rBV	376452	501969	5.51%	0.847%
29	13.985	1039	1041	1043	rBV	1784810	1613174	17.70%	2.721%
30	15.403	1163	1165	1168	rBV	1015409	1456164	15.97%	2.456%

Sum of corrected areas: 59289337

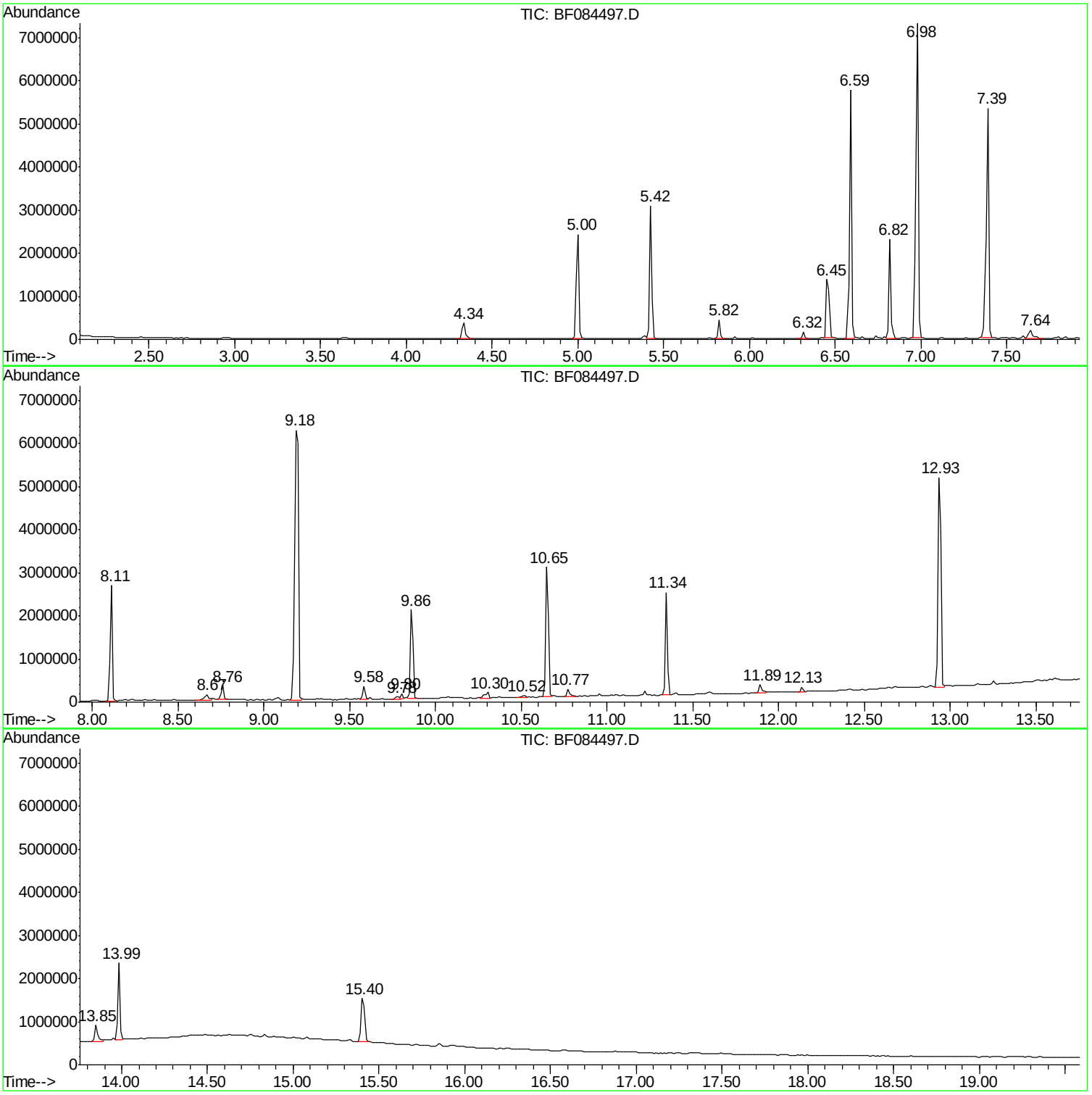
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

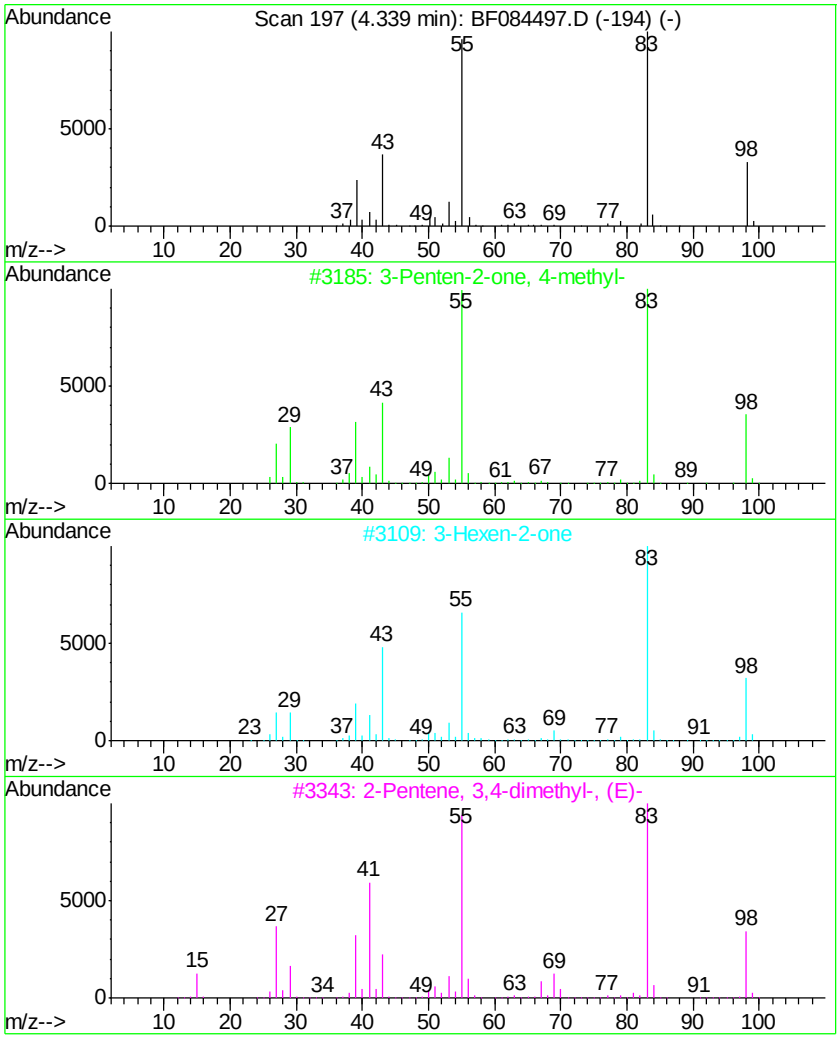
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

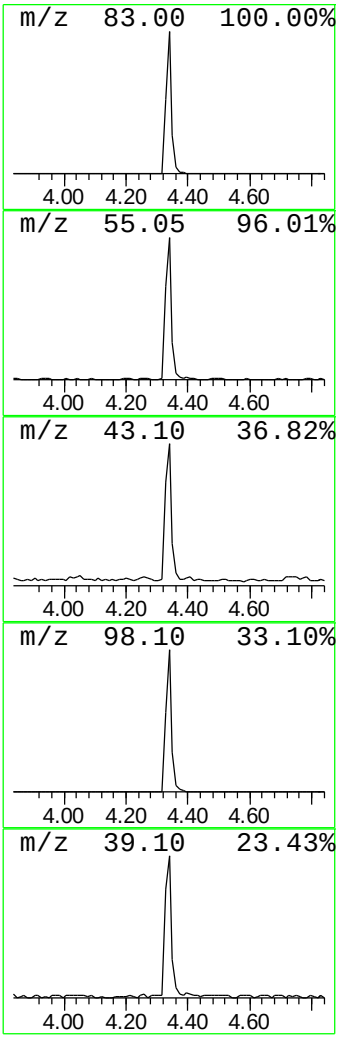
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.34	4.87 ng	492019	1,4-Dichlorobenzene-d4	6.82

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	90
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\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

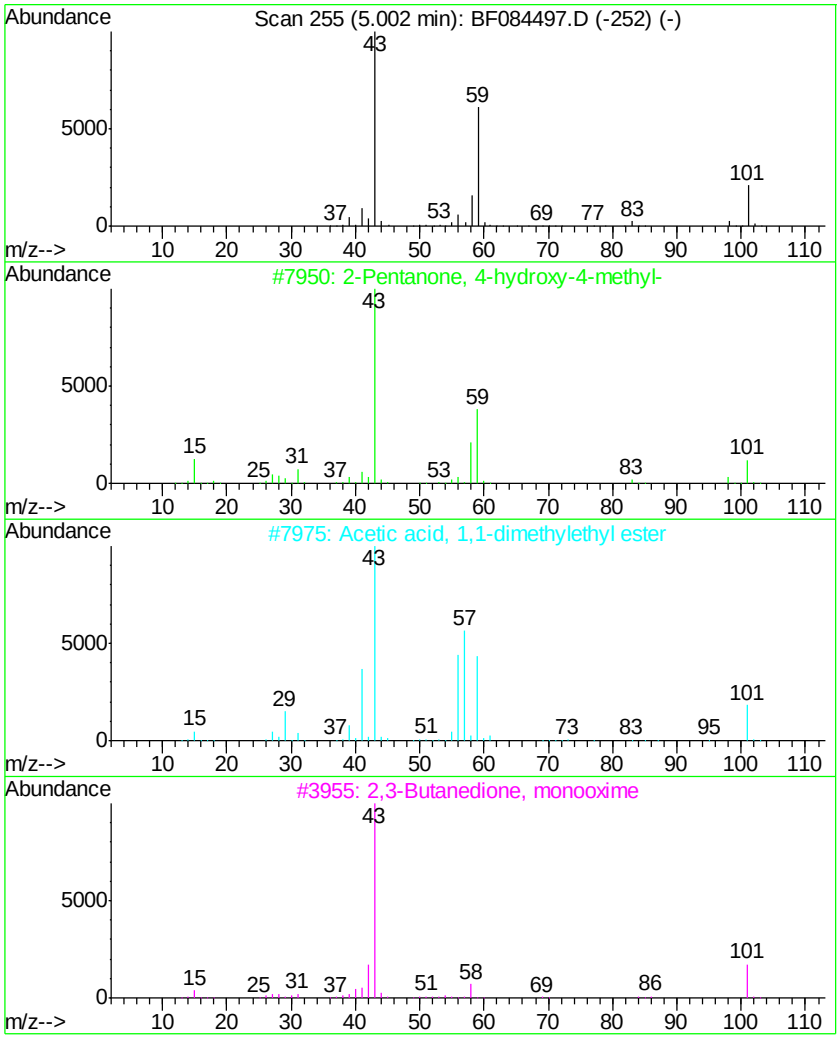
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

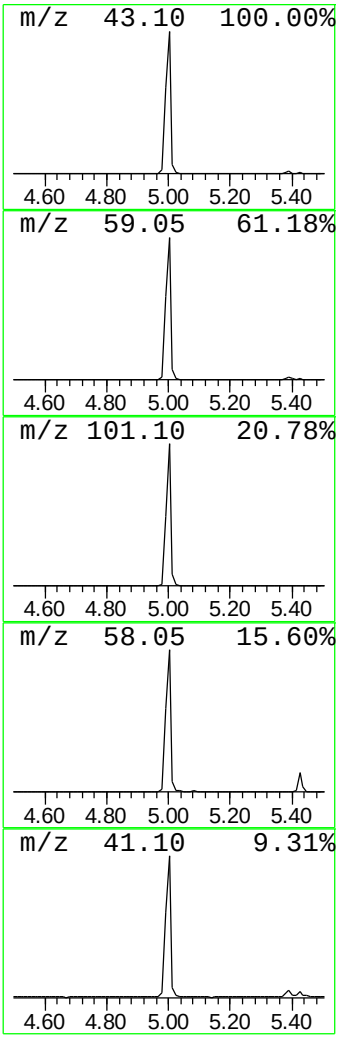
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	27.35 ng	2764640	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

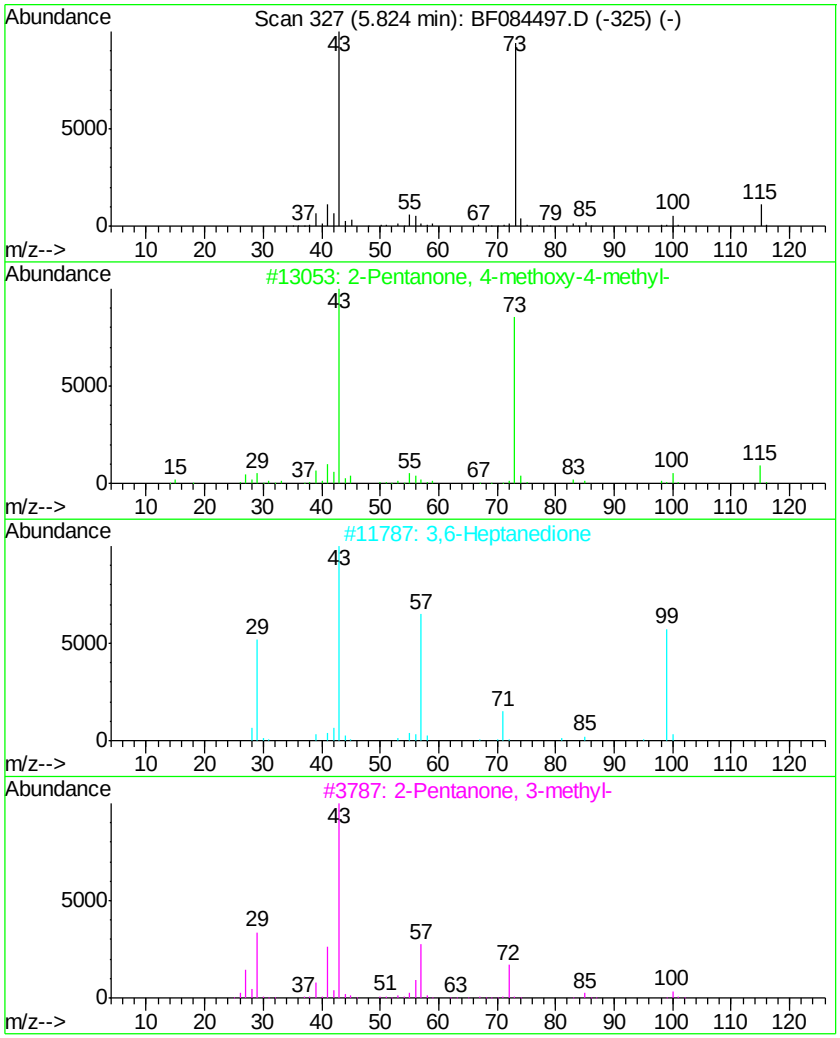
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

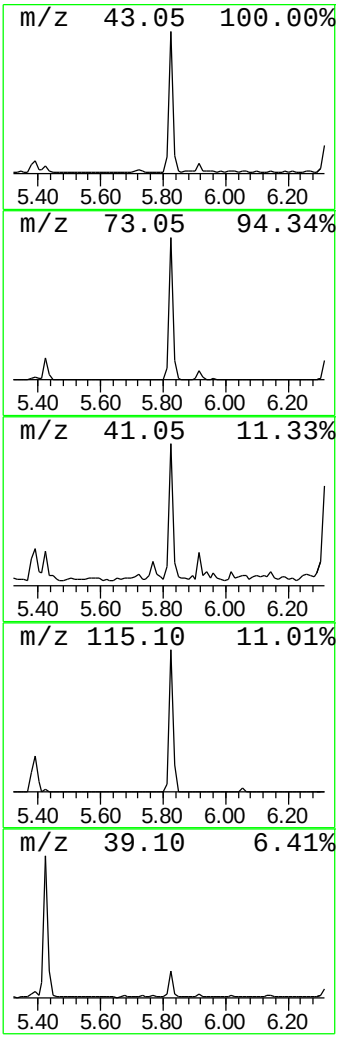
****

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	3.76 ng	380474	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	3,6-Heptanedione	128	C7H12O2	001703-51-1	17
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

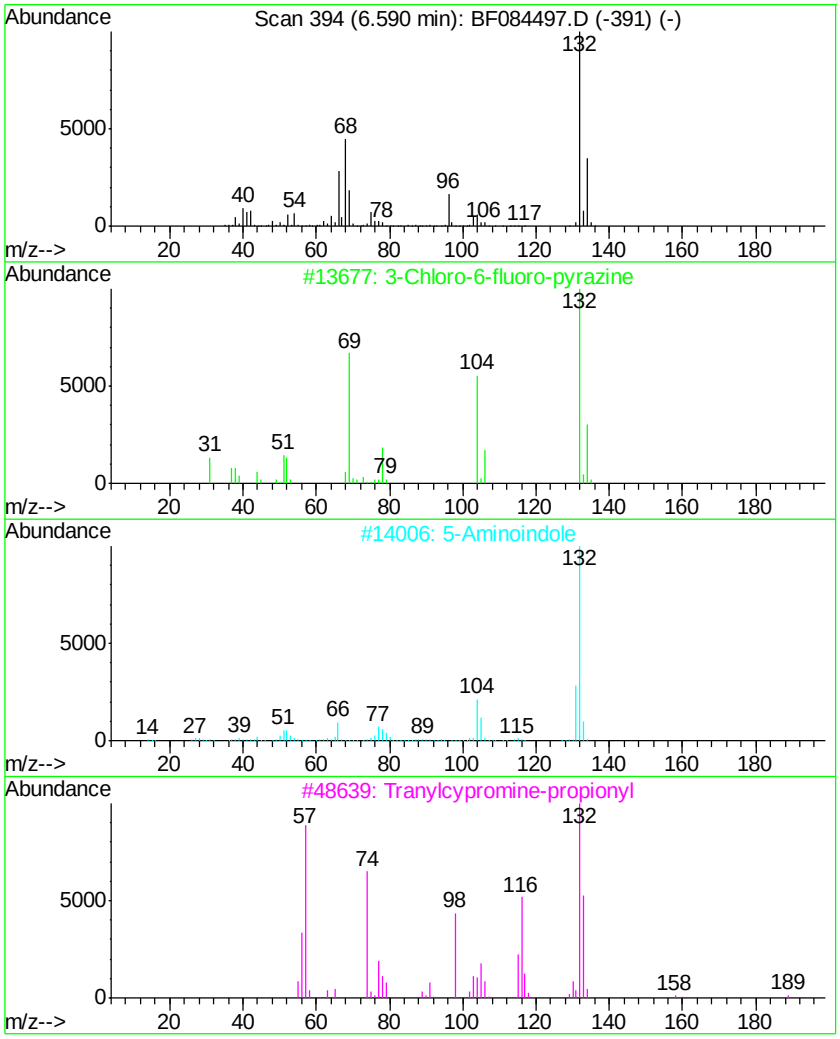
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

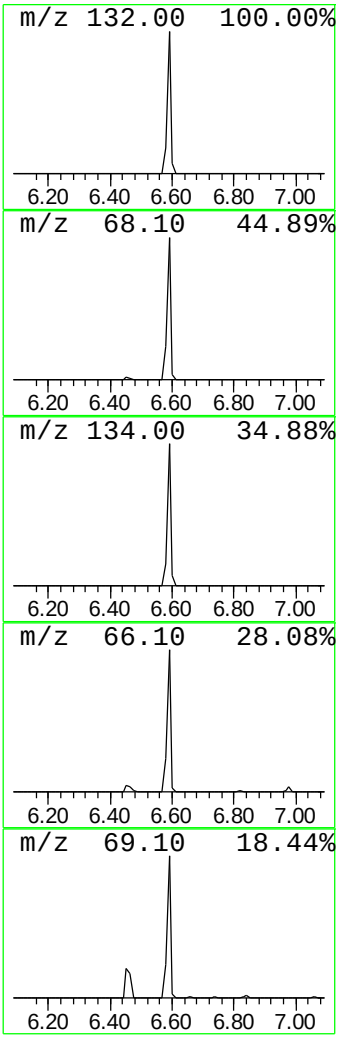
****

Peak Number 4 unknown6.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	49.54 ng	5006460	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

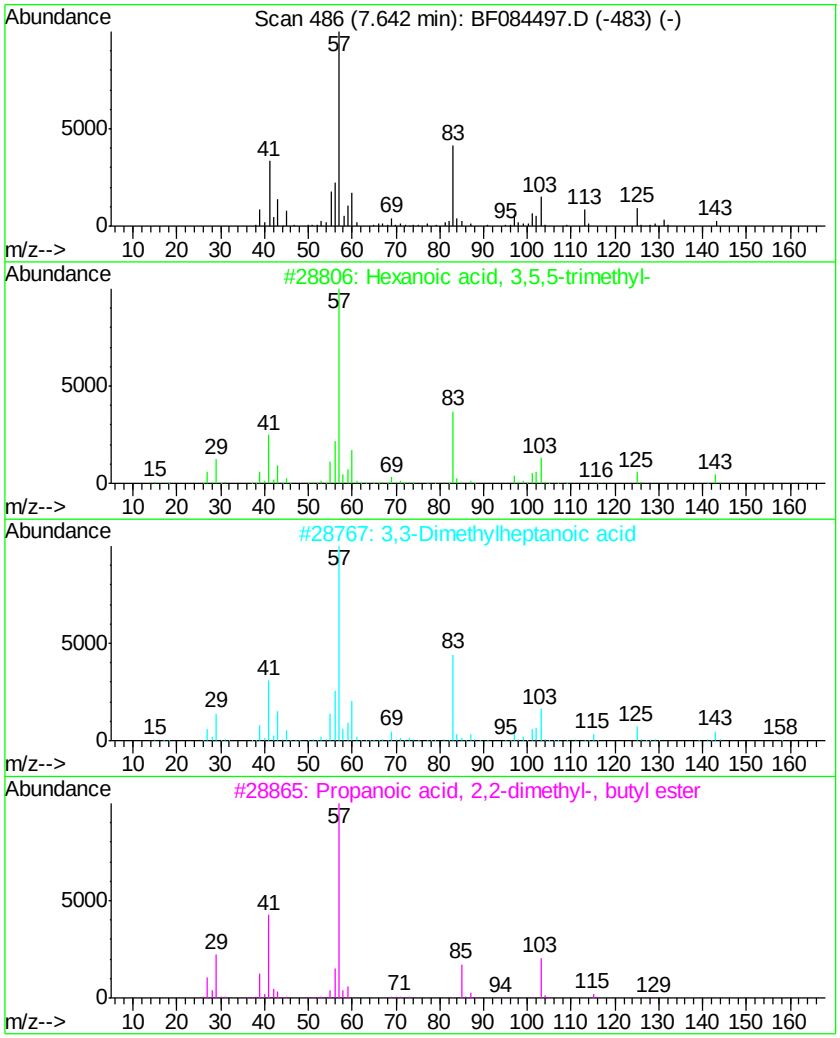
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

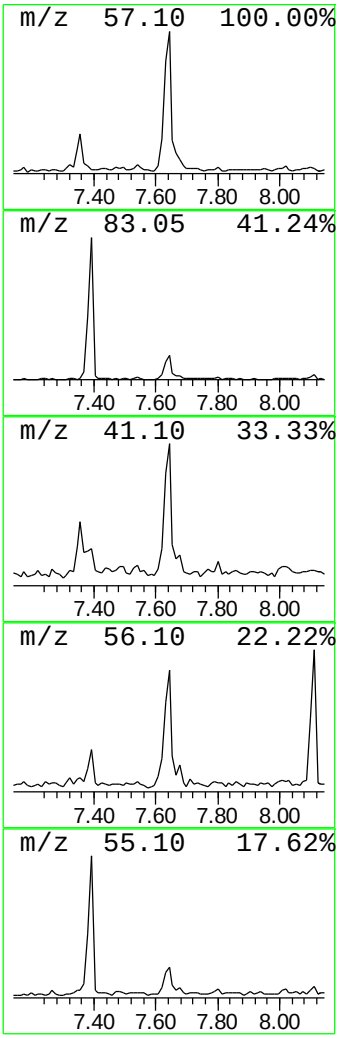
****

Peak Number 6 Hexanoic acid, 3,5,5-trimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	2.67 ng	330152	Naphthalene-d8	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	86
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	47
3	Propanoic acid, 2,2-dimethyl-, b...	158	C9H18O2	005129-37-3	25
4	Octane, 3-methyl-	128	C9H20	002216-33-3	14
5	2,2,4,4-Tetramethyloctane	170	C12H26	062183-79-3	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

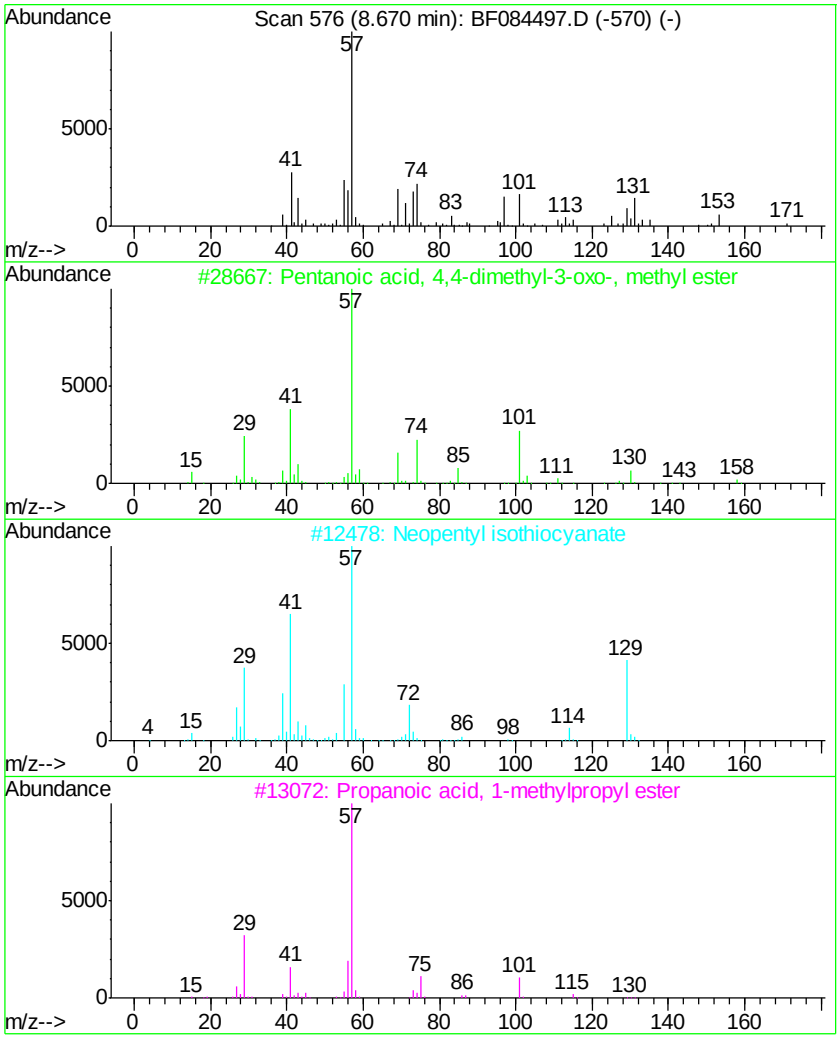
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

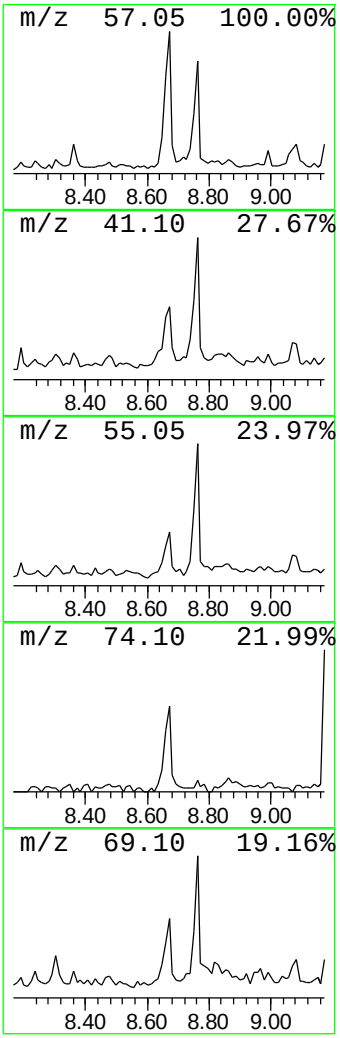
****

Peak Number 7 unknown8.67 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.67	2.49 ng	308313	Naphthalene-d8	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 4,4-dimethyl-3-o...	158	C8H14O3	055107-14-7	37
2	Neopentyl isothiocyanate	129	C6H11NS	000597-97-7	14
3	Propanoic acid, 1-methylpropyl e...	130	C7H14O2	000591-34-4	12
4	1,4-Naphthalenedione	158	C10H6O2	000130-15-4	11
5	3,4-Epoxyhexanoic acid, ethyl ester	158	C8H14O3	061454-92-0	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

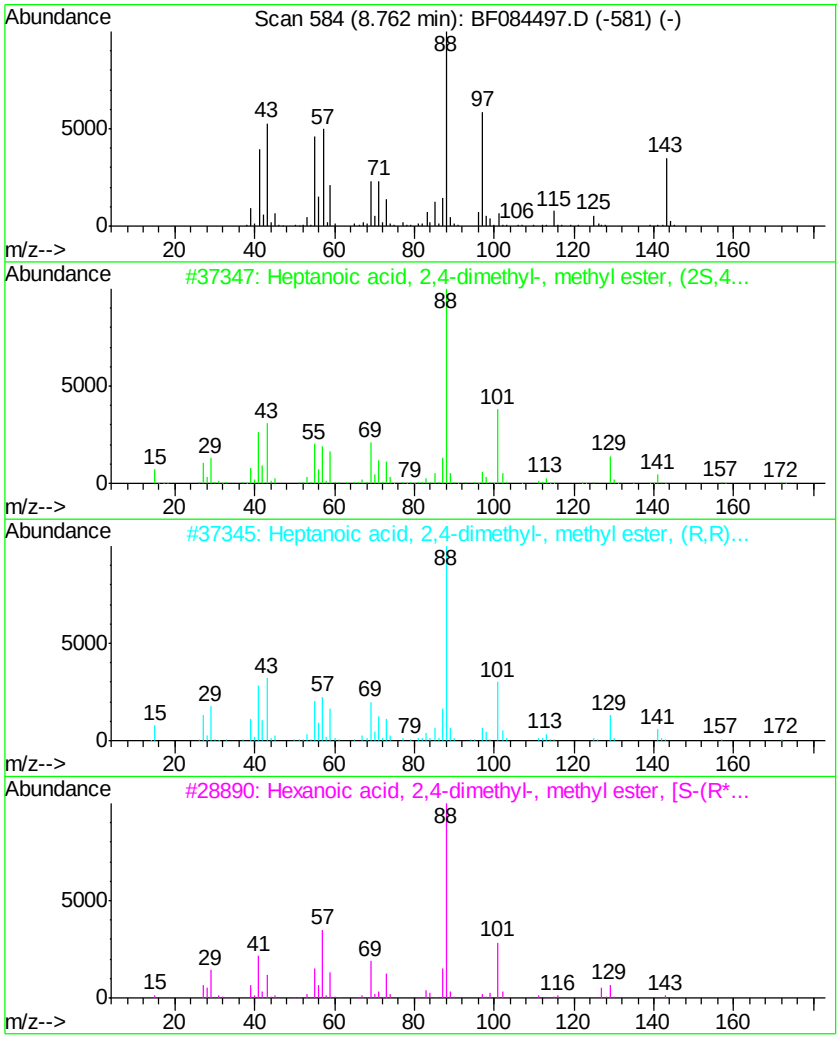
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

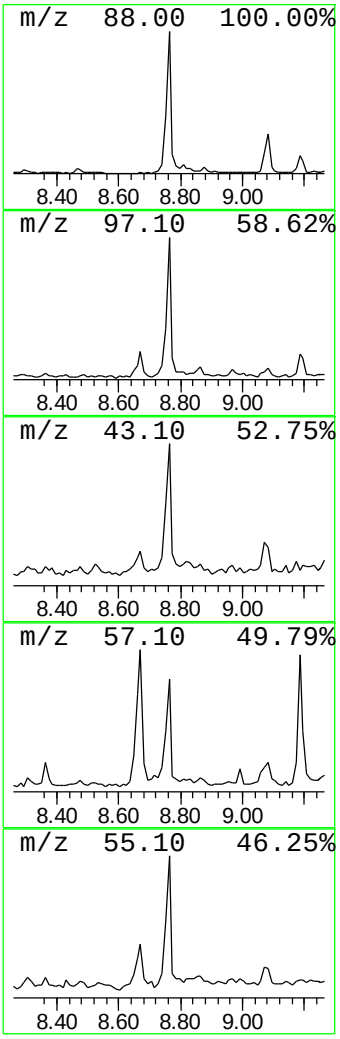
****

Peak Number 8 unknown8.76 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	3.02 ng	373300	Naphthalene-d8	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid, 2,4-dimethyl-, m...	172	C10H20O2	018450-78-7	47
2	Heptanoic acid, 2,4-dimethyl-, m...	172	C10H20O2	018524-86-2	47
3	Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-45-7	43
4	Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	43
5	Butanoic acid, 2,3-dimethyl-, me...	130	C7H14O2	030540-29-5	38





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Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

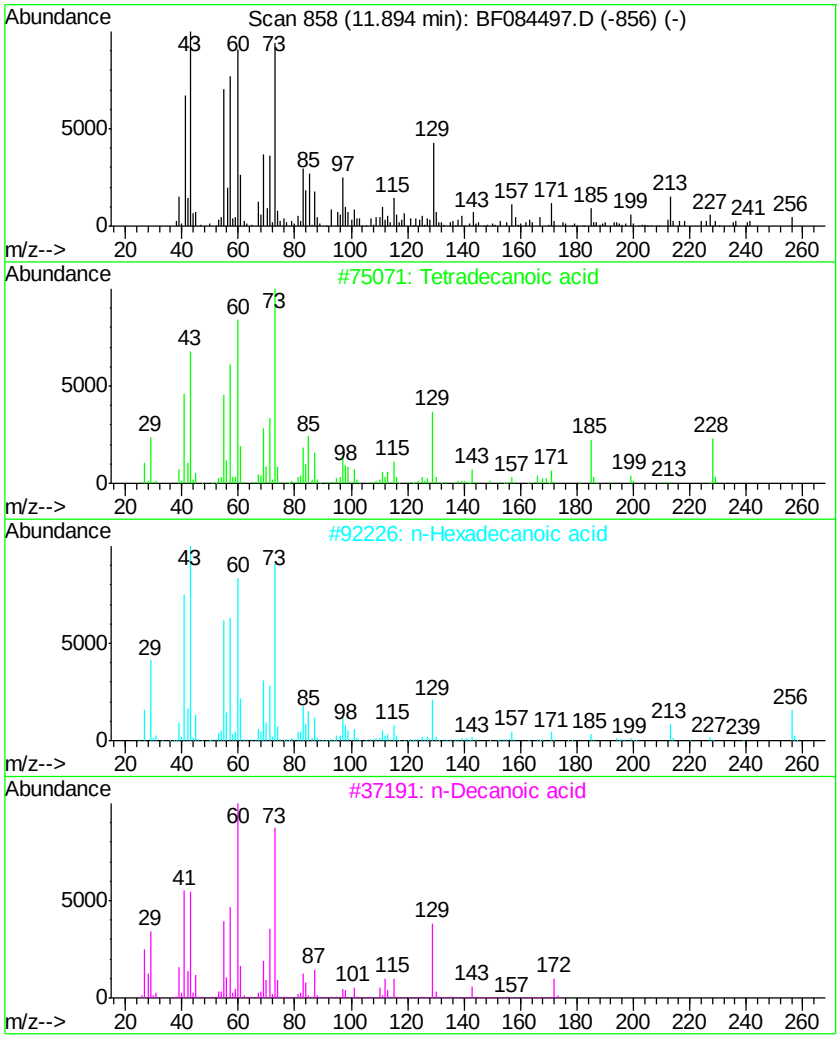
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

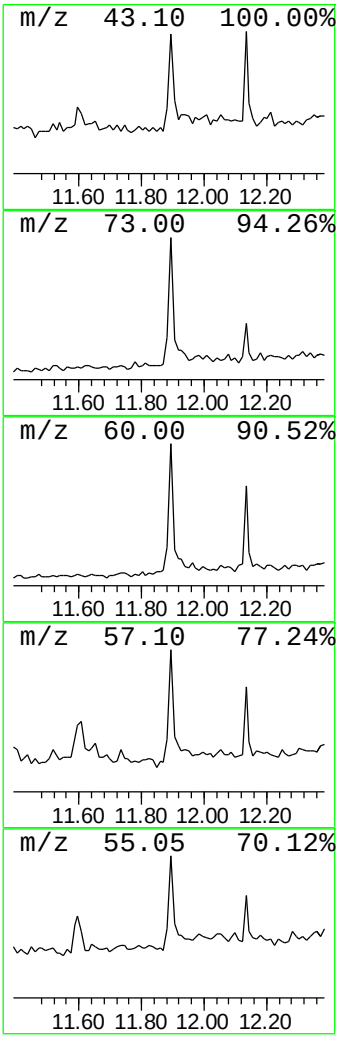
****

Peak Number 9 Tetradecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	2.30 ng	245331	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

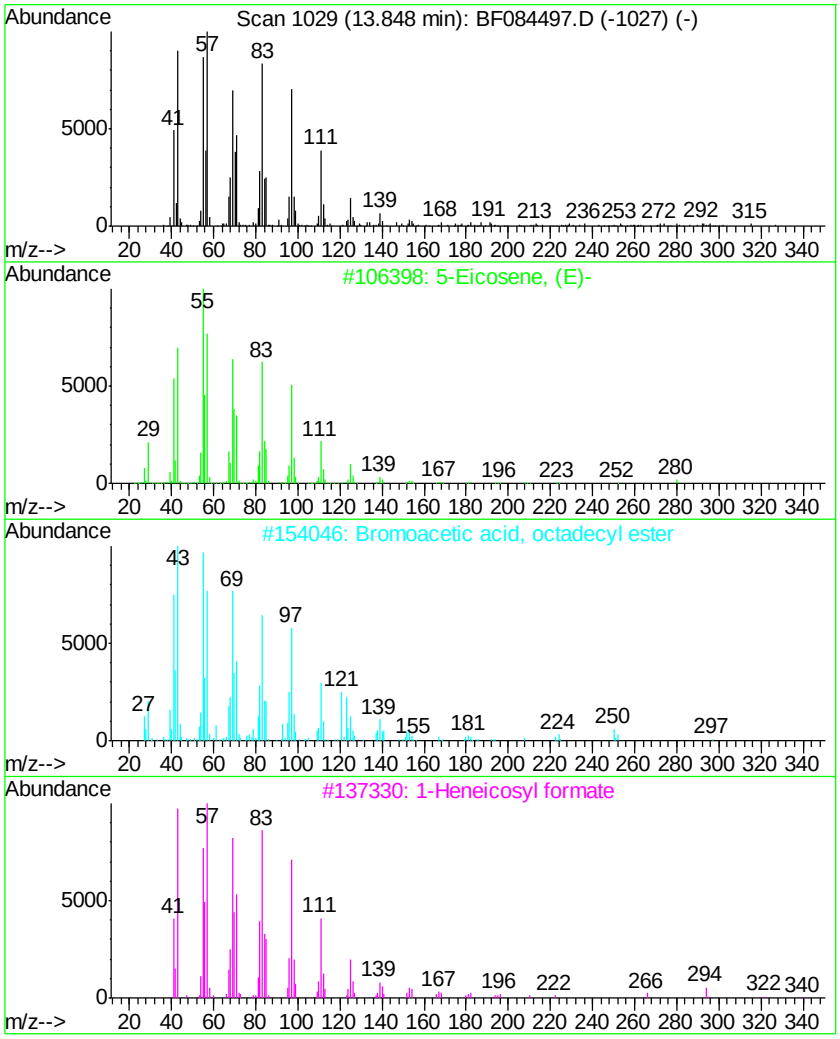
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

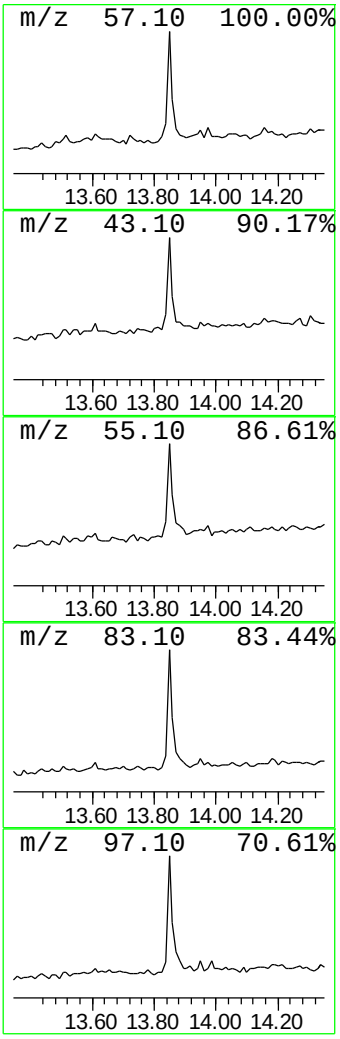
****

Peak Number 10 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	6.22 ng	501969	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	1-Nonadecene	266	C19H38	018435-45-5	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011516\
Data File : BF084497.D
Acq On : 15 Jan 2016 18:10
Operator : SJ/UM
Sample : H1141-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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, 4...	4.34	4.9	ng	492019	1	6.82	2021340	20.0
2-Pentanone, 4-hy...	5.00	27.4	ng	2764640	1	6.82	2021340	20.0
2-Pentanone, 4-me...	5.82	3.8	ng	380474	1	6.82	2021340	20.0
unknown6.59	6.59	49.5	ng	5006460	1	6.82	2021340	20.0
Hexanoic acid, 3,...	7.64	2.7	ng	330152	2	8.11	2475310	20.0
unknown8.67	8.67	2.5	ng	308313	2	8.11	2475310	20.0
unknown8.76	8.76	3.0	ng	373300	2	8.11	2475310	20.0
Tetradecanoic acid	11.89	2.3	ng	245331	4	11.35	2132220	20.0
5-Eicosene, (E)-	13.85	6.2	ng	501969	5	13.99	1613170	20.0