LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090435.D
Acq On : 6 Oct 2016 23:04
Operator : UM/SJ
Sample : H5121-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-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-BF100516.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	4.577	193	196	198	rBV	834036	1087259	12.81%	1.666%
2	5.206	247	251	259	rVB	1863361	2612913	30.80%	4.004%
3	5.606	283	286	289	rBV	5613898	6431201	75.80%	9.855%
4	5.686	291	293	294	rVB	118033	148255	1.75%	0.227%
5	6.623	372	375	377	rBV	6275028	7065130	83.27%	10.827%
6	6.760	384	387	390	rBV	5743249	6760376	79.68%	10.360%
7	6.989	405	407	410	rBV	1005354	1262529	14.88%	1.935%
8	7.149	419	421	423	rVB	4640417	5007242	59.01%	7.673%
9	7.560	454	457	459	rBV	4390582	4883219	57.55%	7.483%
10	8.280	518	520	522	rBV	2094190	1797266	21.18%	2.754%
11	9.366	612	615	617	rBV	8619351	8484708	100.00%	13.002%
12	9.755	646	649	651	rBV	1811690	1495922	17.63%	2.292%
13	10.040	672	674	677	rVB	2226551	1942749	22.90%	2.977%
14	10.829	740	743	746	rBV2	3114877	4553303	53.66%	6.977%
15	10.943	751	753	756	rBV	71662	117637	1.39%	0.180%
16	11.401	791	793	794	rBV	116295	102761	1.21%	0.157%
17	11.538	802	805	807	rBV	1446361	1787015	21.06%	2.738%
18	12.052	848	850	859	rBV	259291	326935	3.85%	0.501%
19	12.841	917	919	926	rBV	124157	177021	2.09%	0.271%
20	13.127	941	944	946	rBV	7221483	6503018	76.64%	9.965%
21	14.018	1020	1022	1032	rBV	367917	440003	5.19%	0.674%
22	14.178	1034	1036	1039	rVB	1350840	1172743	13.82%	1.797%
23	15.675	1164	1167	1170	rBV	700076	1098415	12.95%	1.683%

Sum of corrected areas: 65257620

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
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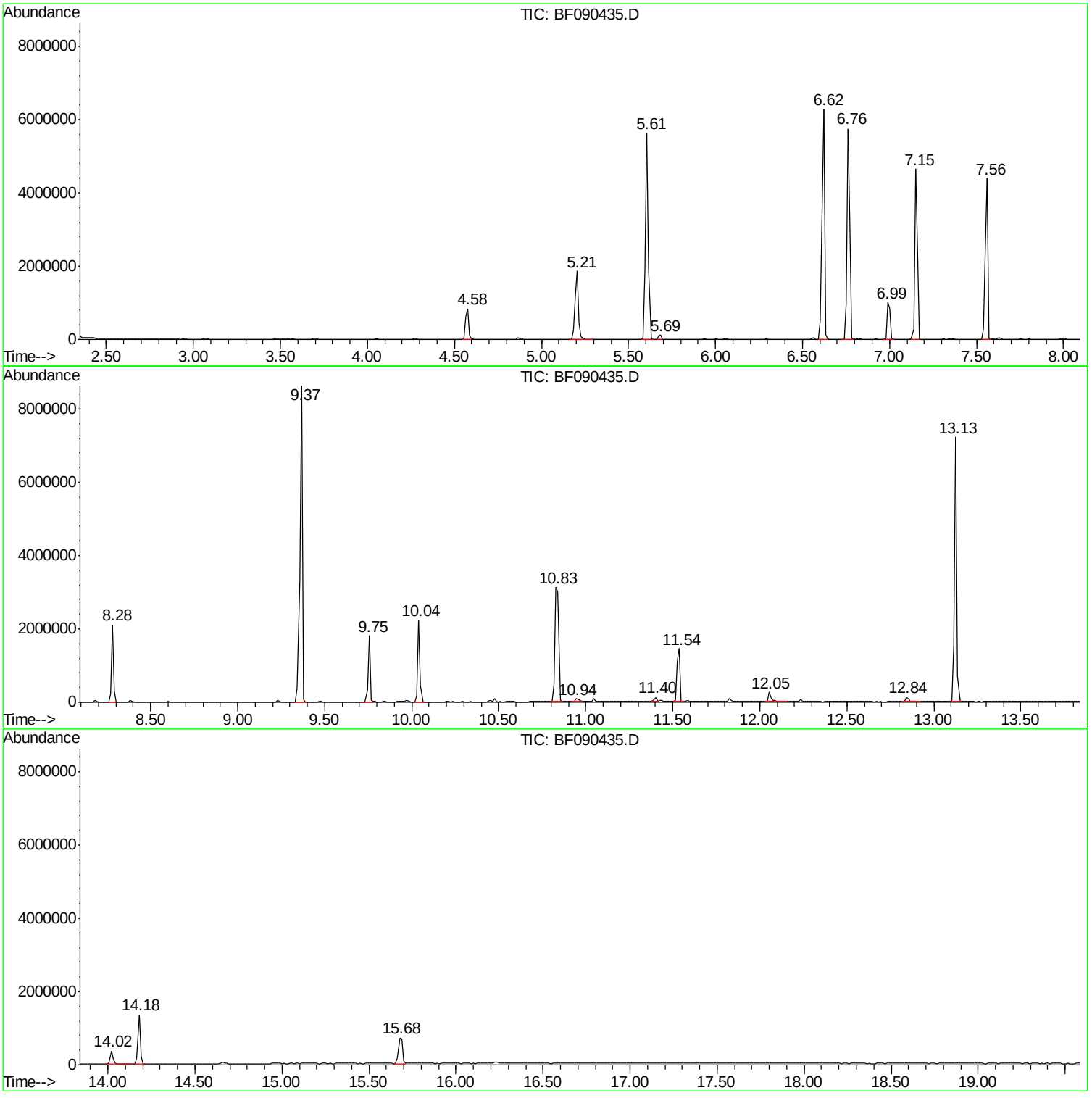
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BF090435.D
Acq On : 6 Oct 2016 23:04
Operator : UM/SJ
Sample : H5121-02
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
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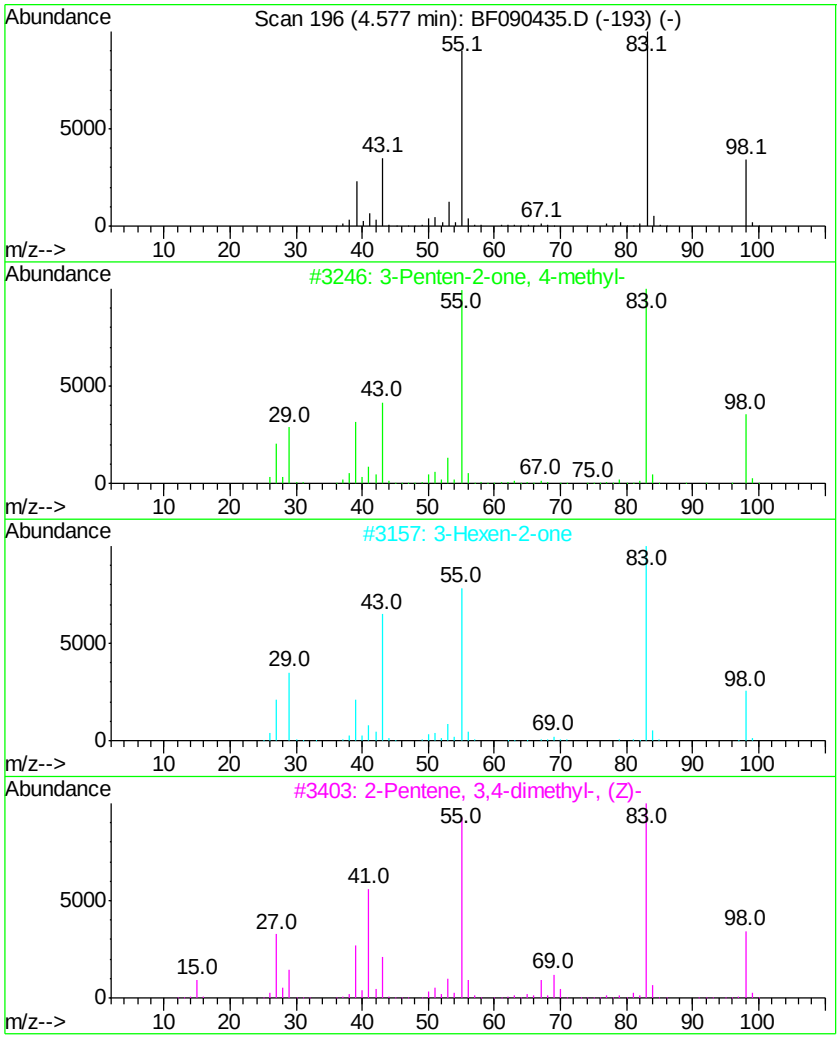
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

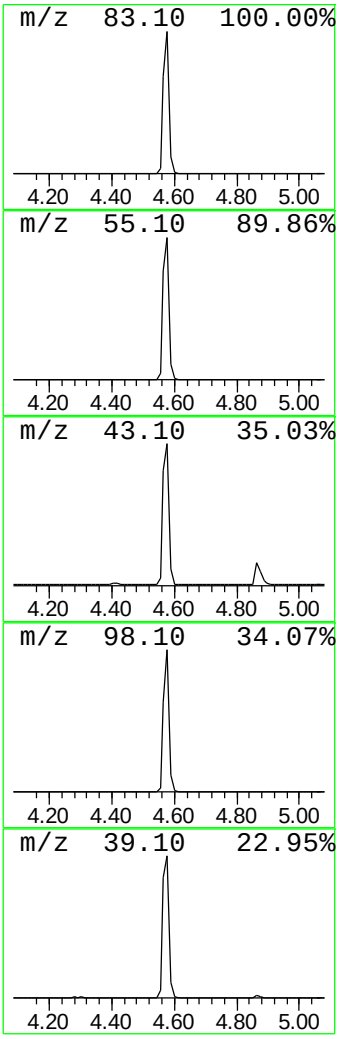
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	17.22 ng	1087260	1,4-Dichlorobenzene-d4	7.00

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-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090435.D
Acq On : 6 Oct 2016 23:04
Operator : UM/SJ
Sample : H5121-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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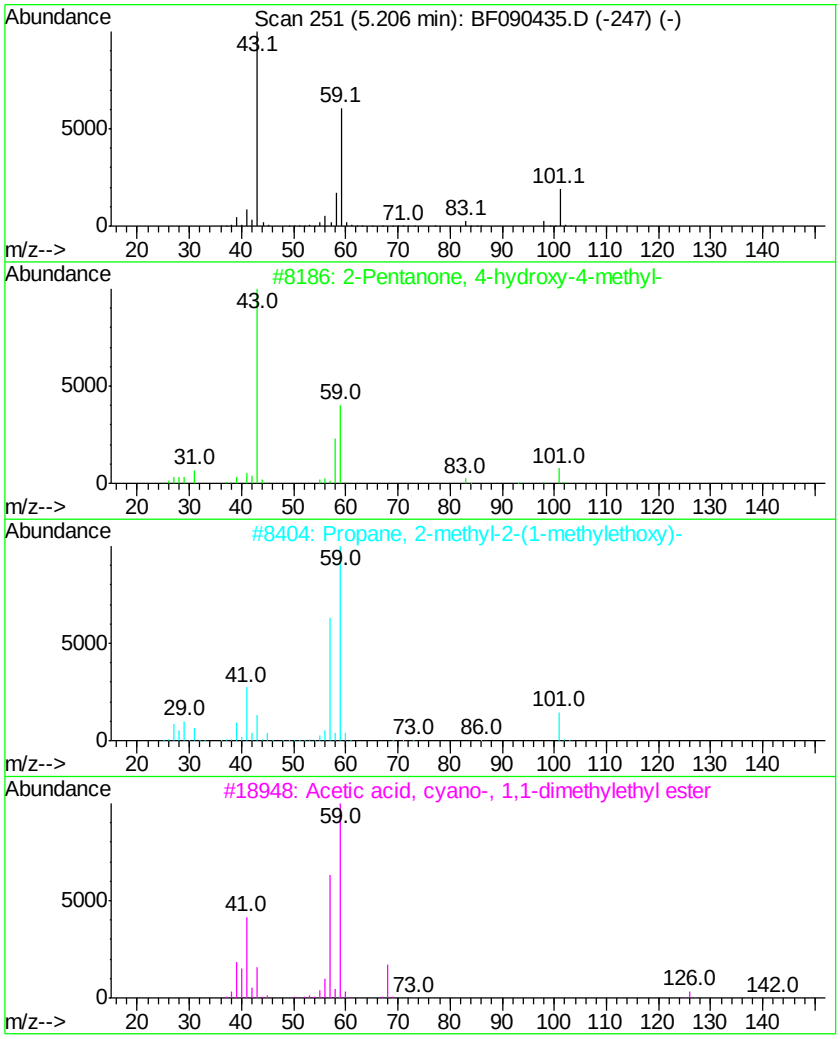
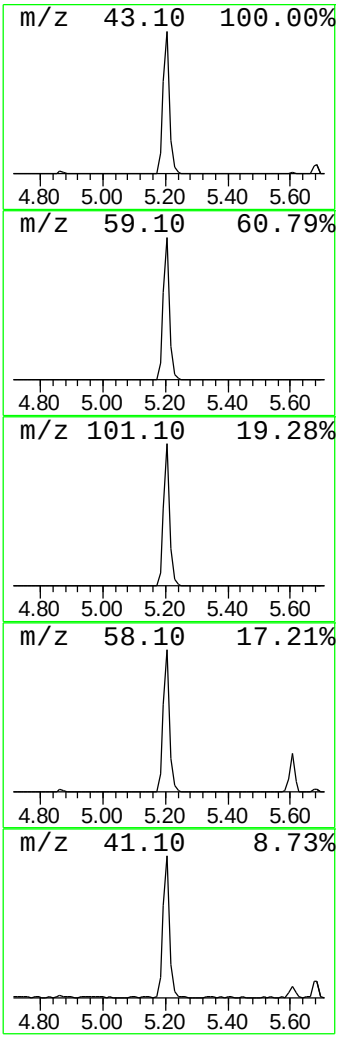
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	41.39 ng	2612910	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Acetone	58	C3H6O	000067-64-1	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090435.D
Acq On : 6 Oct 2016 23:04
Operator : UM/SJ
Sample : H5121-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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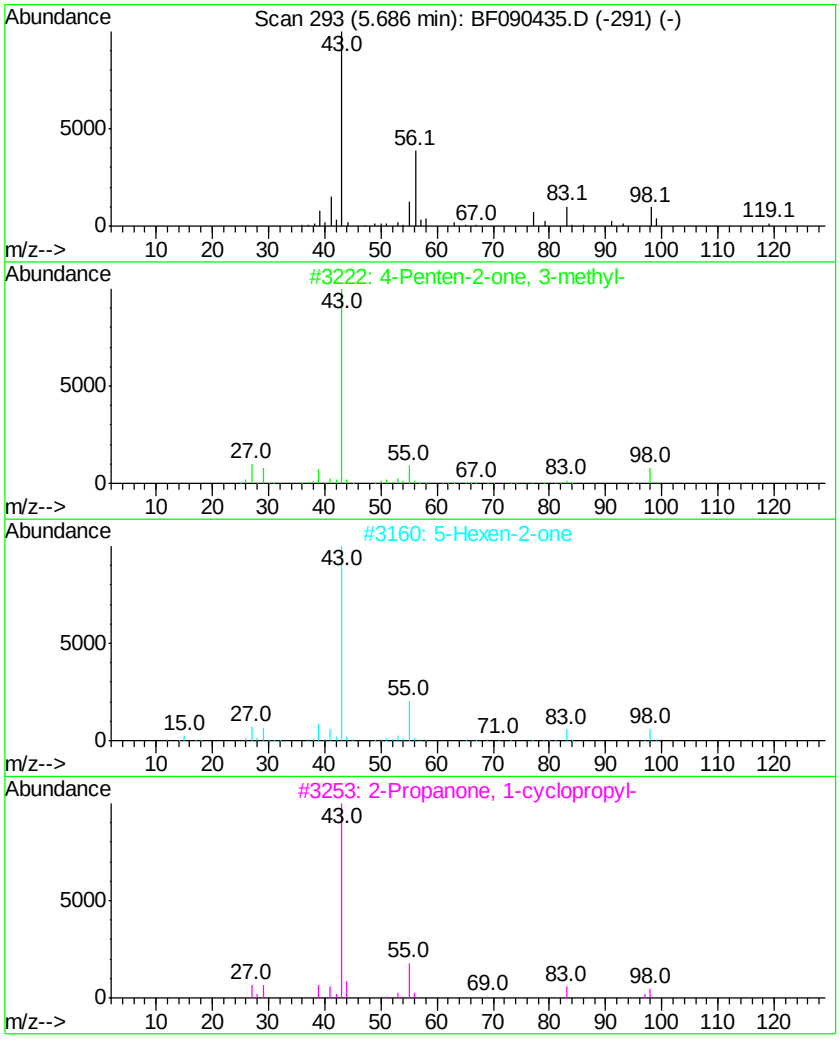
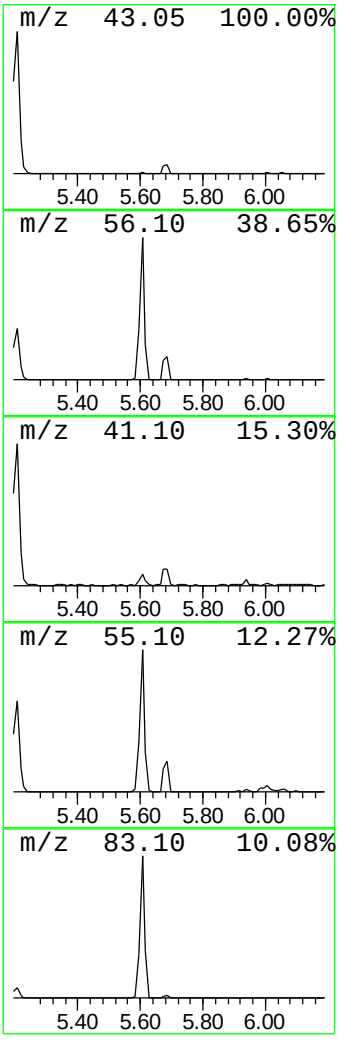
Peak Number 3 unknown5.69 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	2.35 ng	148255	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	22
2	5-Hexen-2-one	98	C6H10O	000109-49-9	12
3	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9
5	Butane, 1-isocyanato-	99	C5H9NO	000111-36-4	9





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Data File : BF090435.D
Acq On : 6 Oct 2016 23:04
Operator : UM/SJ
Sample : H5121-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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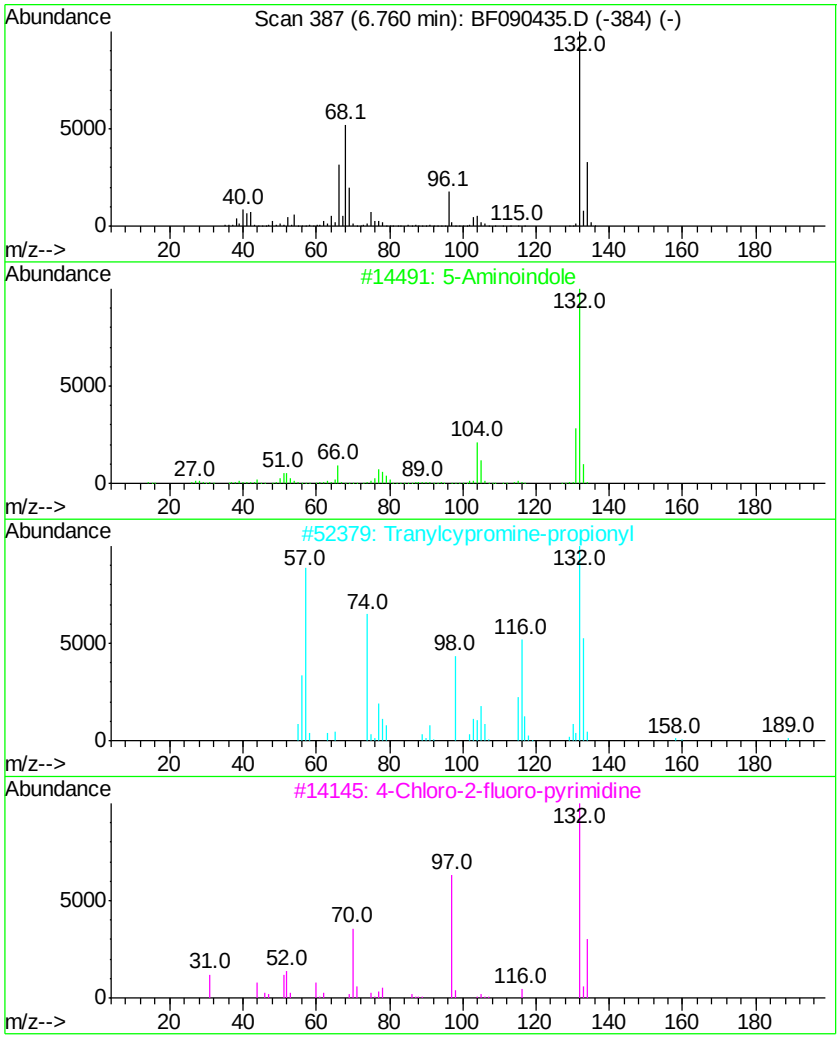
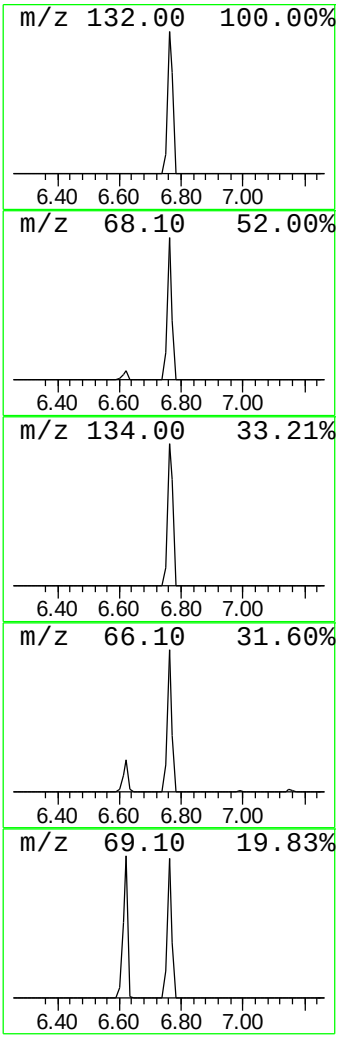
Peak Number 4 unknown6.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	107.09 ng	6760380	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
Data File : BF090435.D
Acq On : 6 Oct 2016 23:04
Operator : UM/SJ
Sample : H5121-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

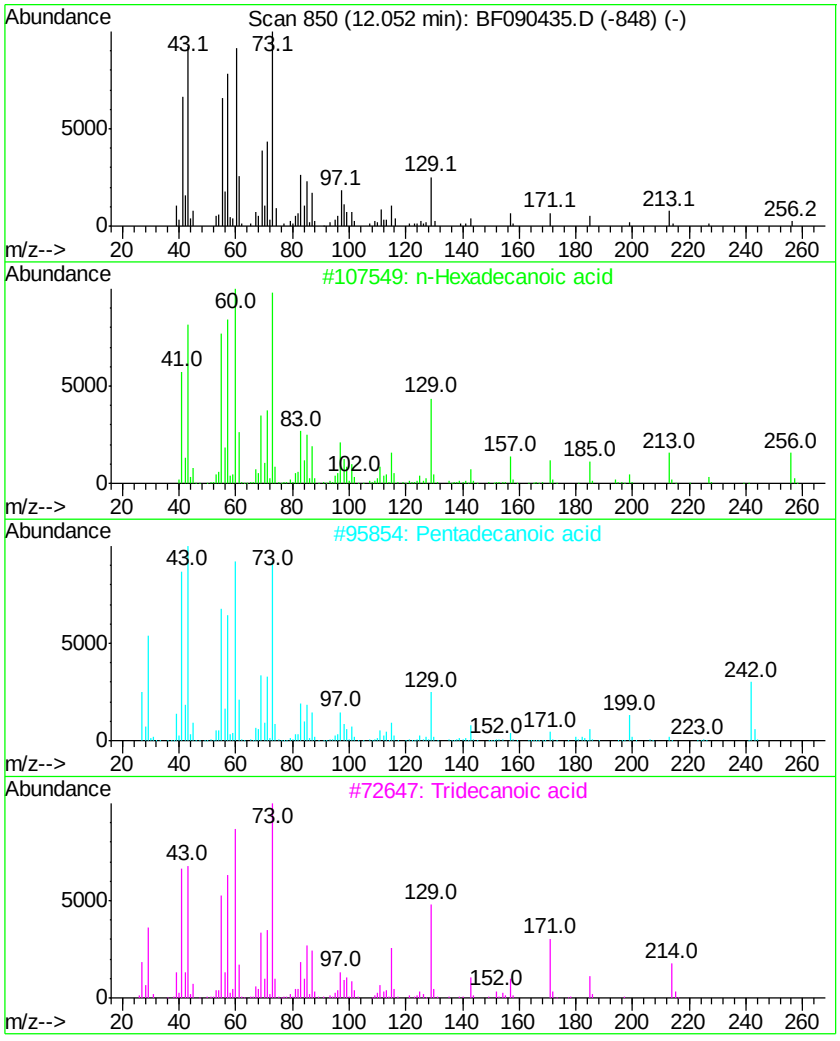
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

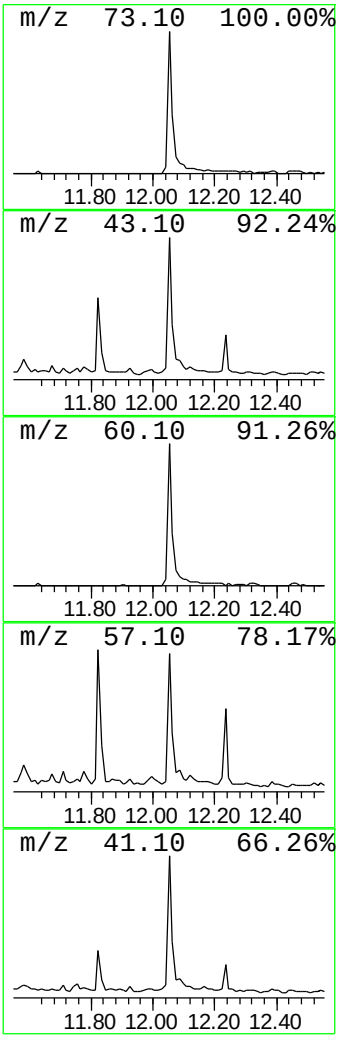
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	3.66 ng	326935	Phenanthrene-d10	11.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\
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Sample : H5121-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

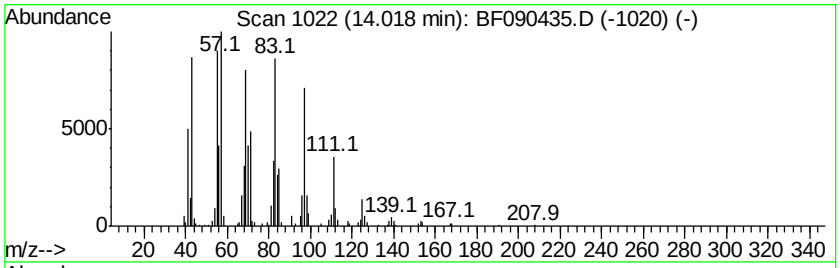
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

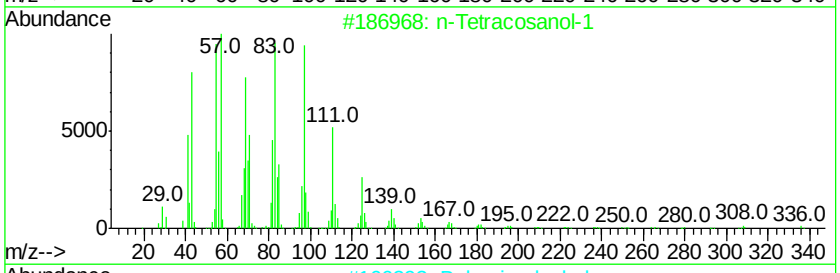
****

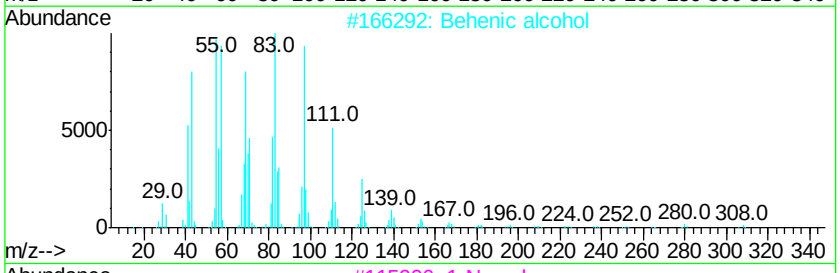
Peak Number 7 n-Tetracosanol-1 Concentration Rank 5

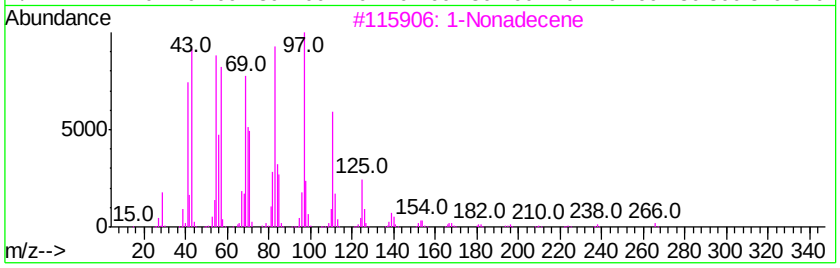
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	7.50 ng	440003	Chrysene-d12	14.18

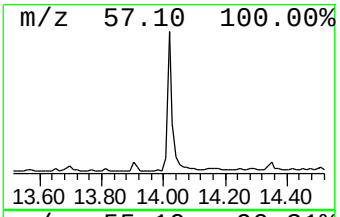
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91

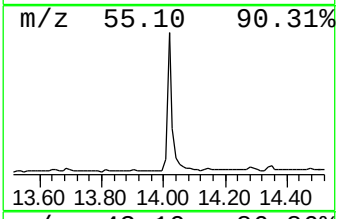


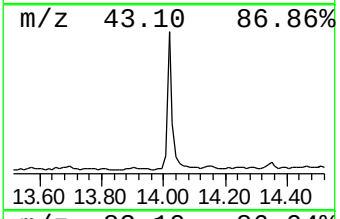


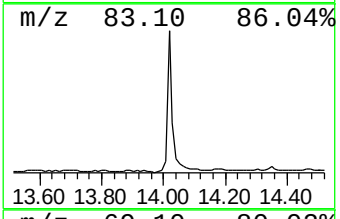


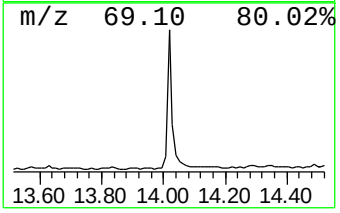












Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.58	17.2	ng	1087260	1	7.00	1262530	20.0
2-Pentanone, 4-hy...	5.21	41.4	ng	2612910	1	7.00	1262530	20.0
unknown5.69	5.69	2.4	ng	148255	1	7.00	1262530	20.0
unknown6.76	6.76	107.1	ng	6760380	1	7.00	1262530	20.0
n-Hexadecanoic acid	12.05	3.7	ng	326935	4	11.54	1787020	20.0
n-Tetracosanol-1	14.02	7.5	ng	440003	5	14.18	1172740	20.0