LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080731.D
Acq On : 31 Jul 2015 13:34
Operator : TP/UM
Sample : PB84695BL
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB84695BL

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-BF073015.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	3.493	120	123	130	rVB	56074	105737	1.46%	0.206%
2	4.430	201	205	208	rBV	3547157	4553359	62.98%	8.893%
3	5.081	256	262	264	rBV	3704556	7229698	100.00%	14.119%
4	5.470	293	296	298	rBV	4264072	4586159	63.44%	8.957%
5	5.870	328	331	333	rBV	399649	364622	5.04%	0.712%
6	6.476	381	384	387	rBV	3037050	4205013	58.16%	8.212%
7	6.624	394	397	399	rBV	3450159	4438320	61.39%	8.668%
8	6.853	414	417	419	rVB	1153963	1006791	13.93%	1.966%
9	7.013	428	431	433	rBV	2604492	3311688	45.81%	6.468%
10	7.413	463	466	468	rBV	2842154	2952313	40.84%	5.766%
11	8.133	526	529	531	rBV	1356374	1282182	17.73%	2.504%
12	9.207	620	623	626	rBV	3566812	4639882	64.18%	9.061%
13	9.882	679	682	685	rBV	1174170	1330744	18.41%	2.599%
14	10.670	748	751	754	rBV	2934394	3016289	41.72%	5.891%
15	11.368	809	812	814	rBV	1559222	1451855	20.08%	2.835%
16	12.785	933	936	938	rBV	145660	192926	2.67%	0.377%
17	12.956	948	951	953	rBV	4151140	4671787	64.62%	9.124%
18	13.482	995	997	999	rBV	199924	162666	2.25%	0.318%
19	13.997	1039	1042	1044	rBV	834038	962353	13.31%	1.879%
20	15.414	1163	1166	1168	rBV	519832	740086	10.24%	1.445%

Sum of corrected areas: 51204470

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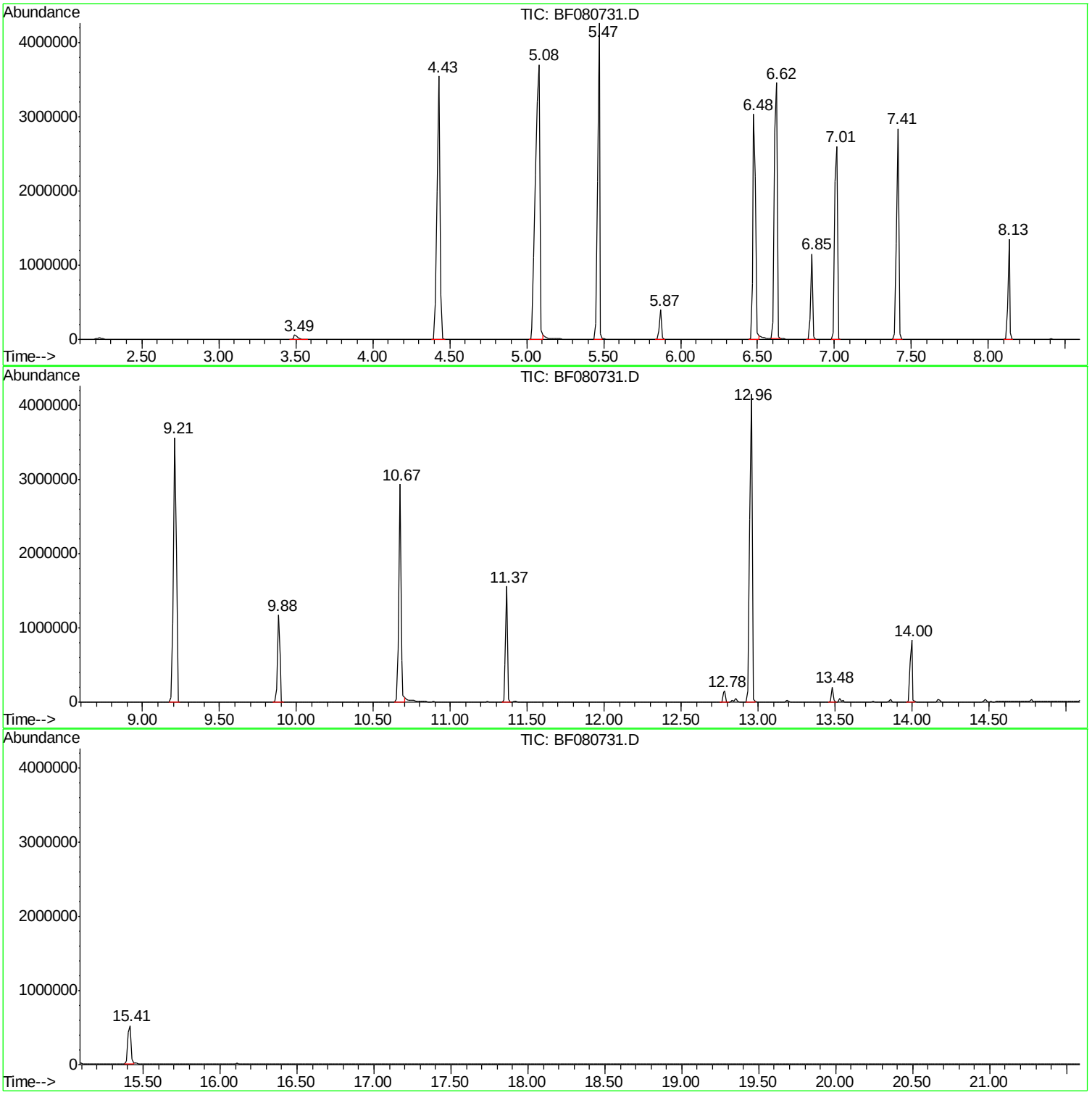
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB84695BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
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Operator : TP/UM
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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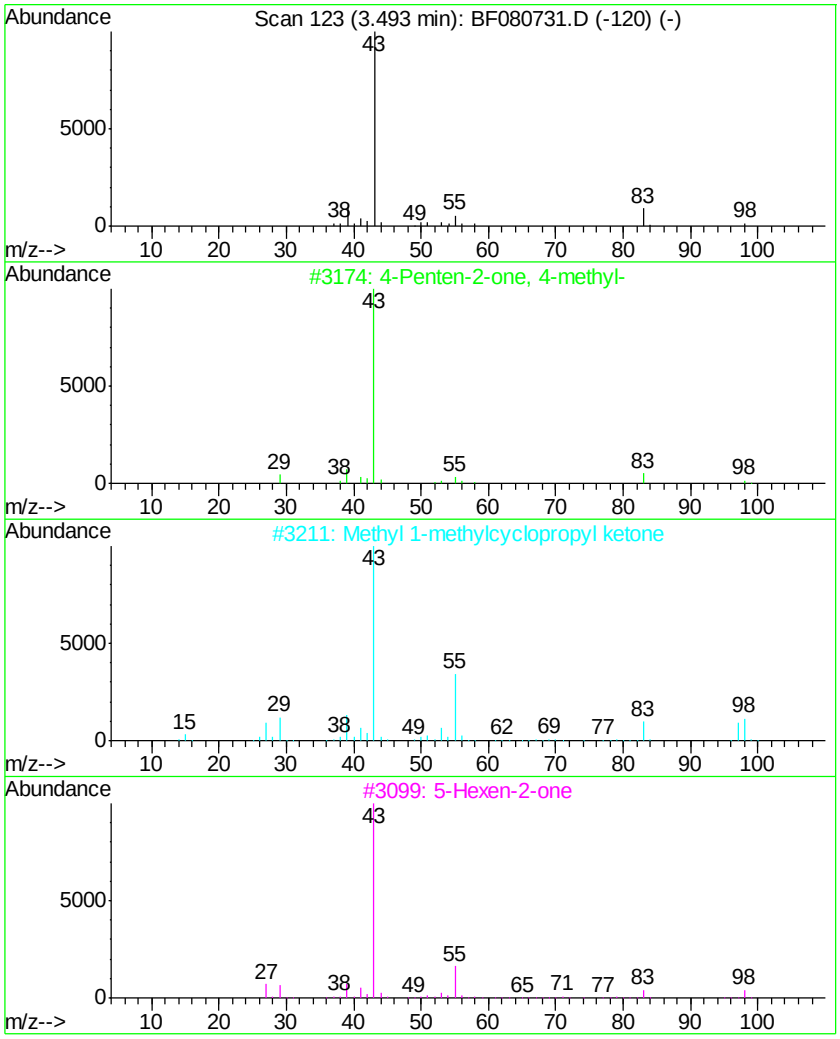
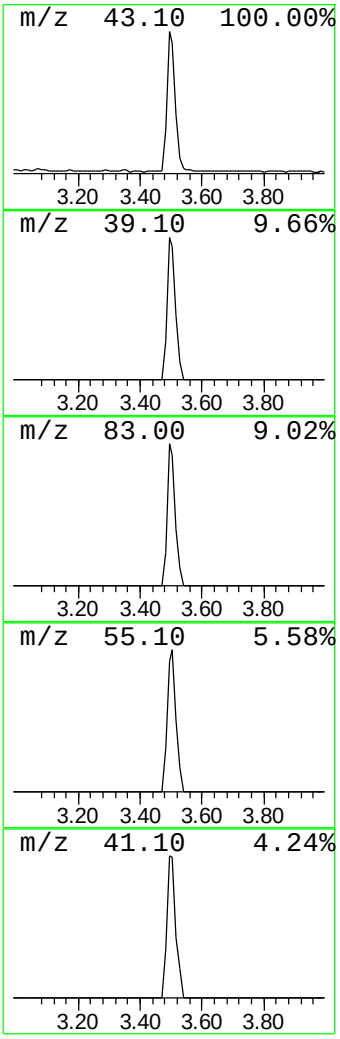
Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.49	2.10 ng	105737	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	43
3	5-Hexen-2-one	98	C6H10O	000109-49-9	43
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9





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Acq On : 31 Jul 2015 13:34
Operator : TP/UM
Sample : PB84695BL
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB84695BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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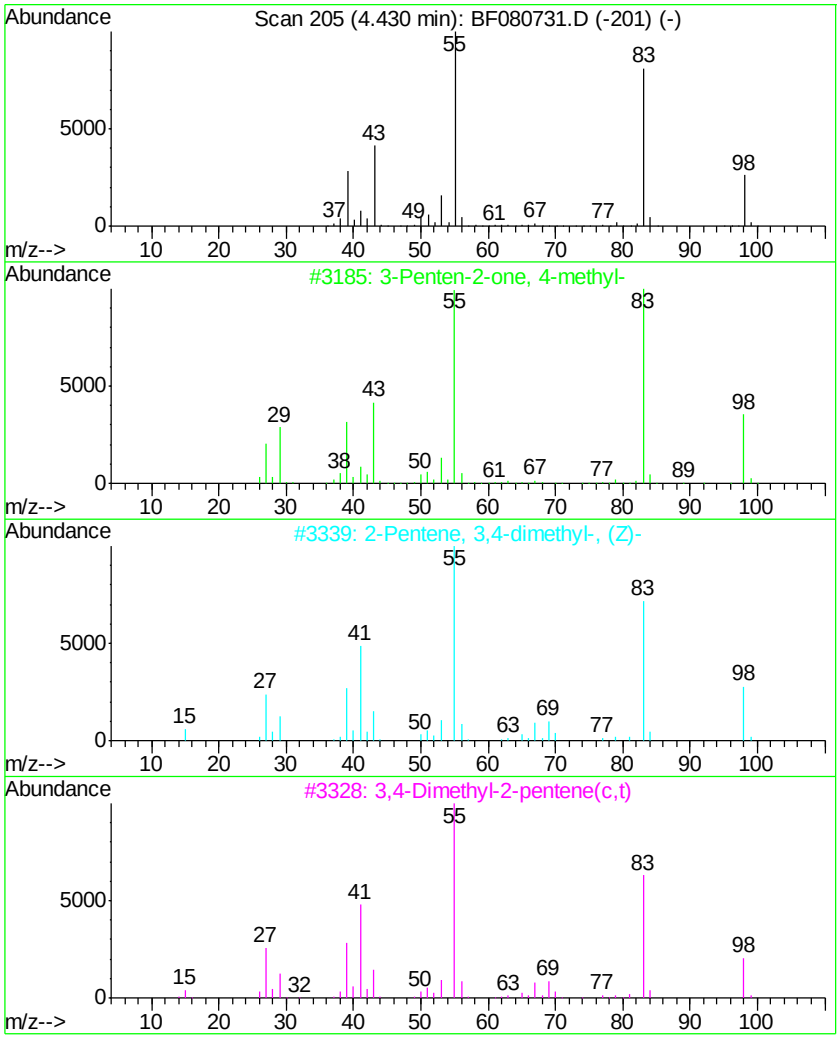
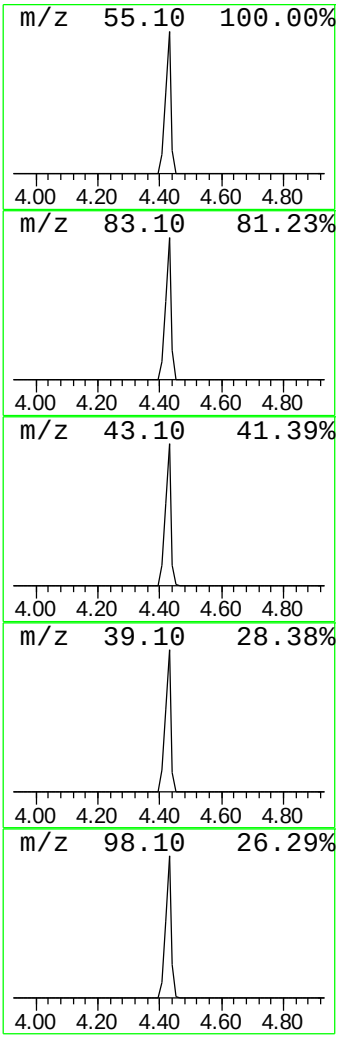
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.43	90.45 ng	4553360	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
3	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
4	3-Hexen-2-one	98	C6H10O	000763-93-9	80
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78





Library Search Compound Report

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Data File : BF080731.D
Acq On : 31 Jul 2015 13:34
Operator : TP/UM
Sample : PB84695BL
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB84695BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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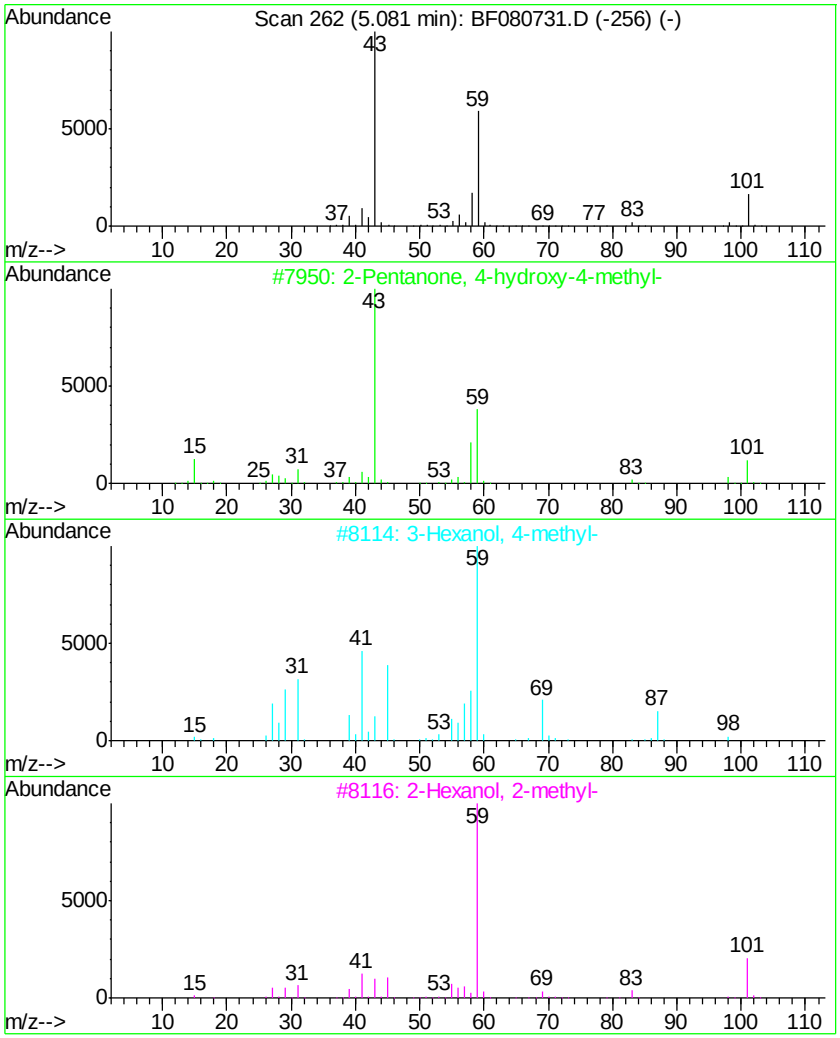
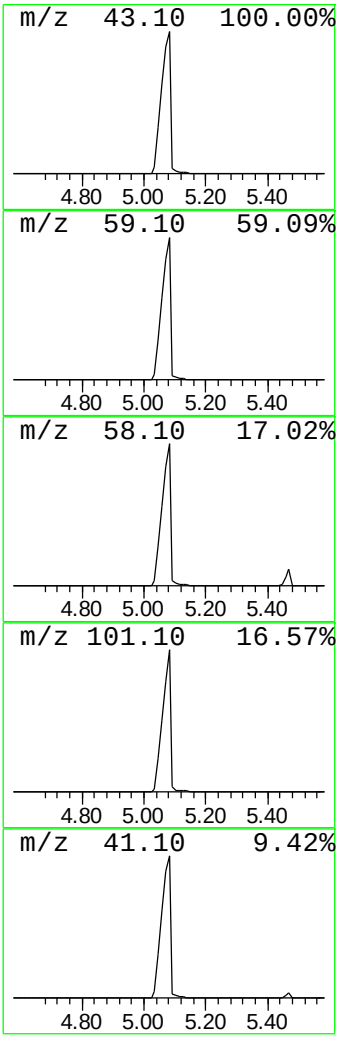
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	143.62 ng	7229700	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Sample : PB84695BL
Misc :
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Instrument : BNA_F
ClientSampleId : PB84695BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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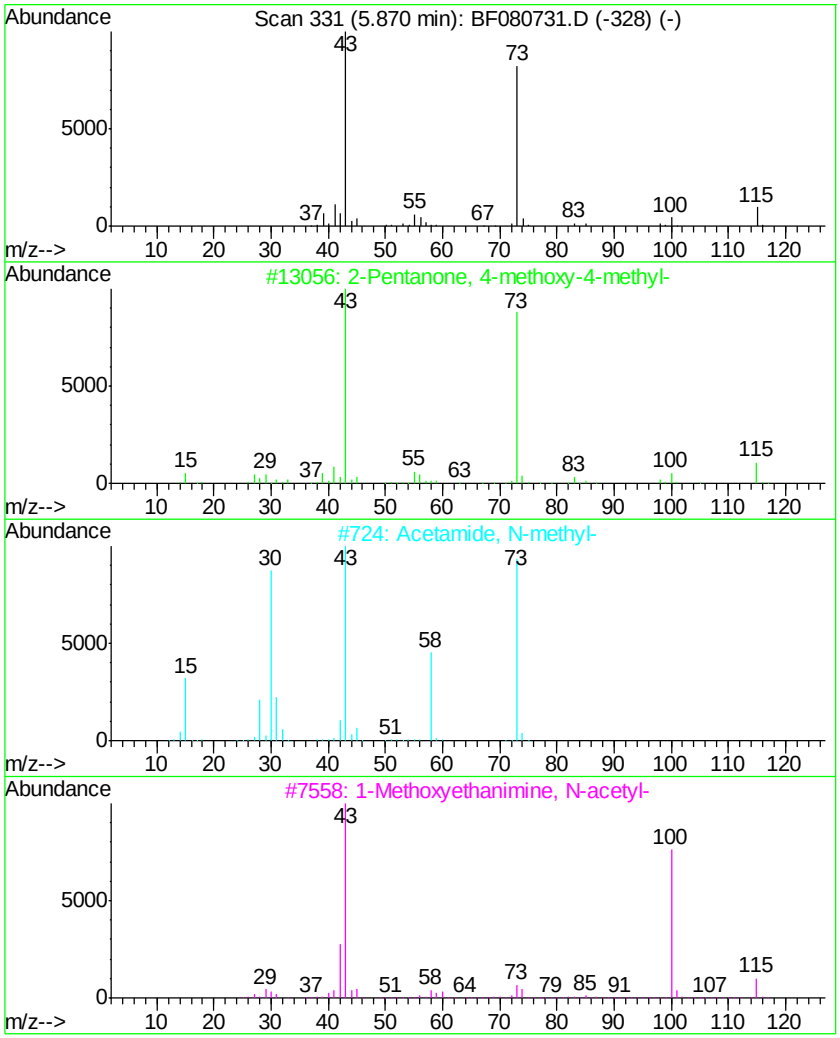
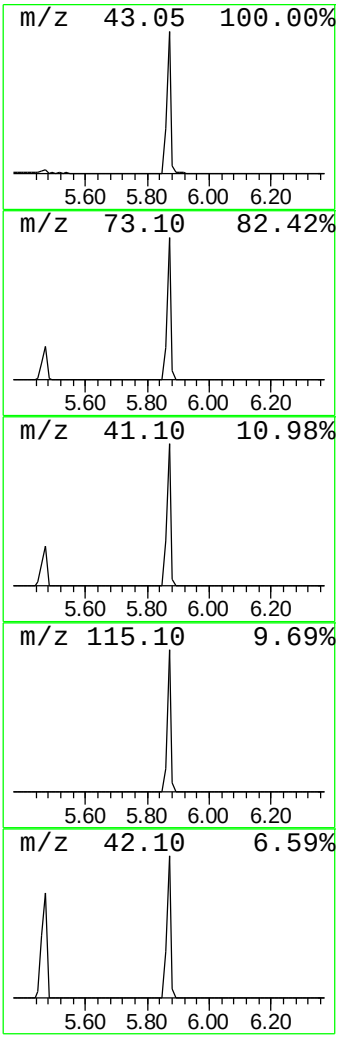
Peak Number 4 unknown5.87 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.87	7.24 ng	364622	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	17
4	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	12
5	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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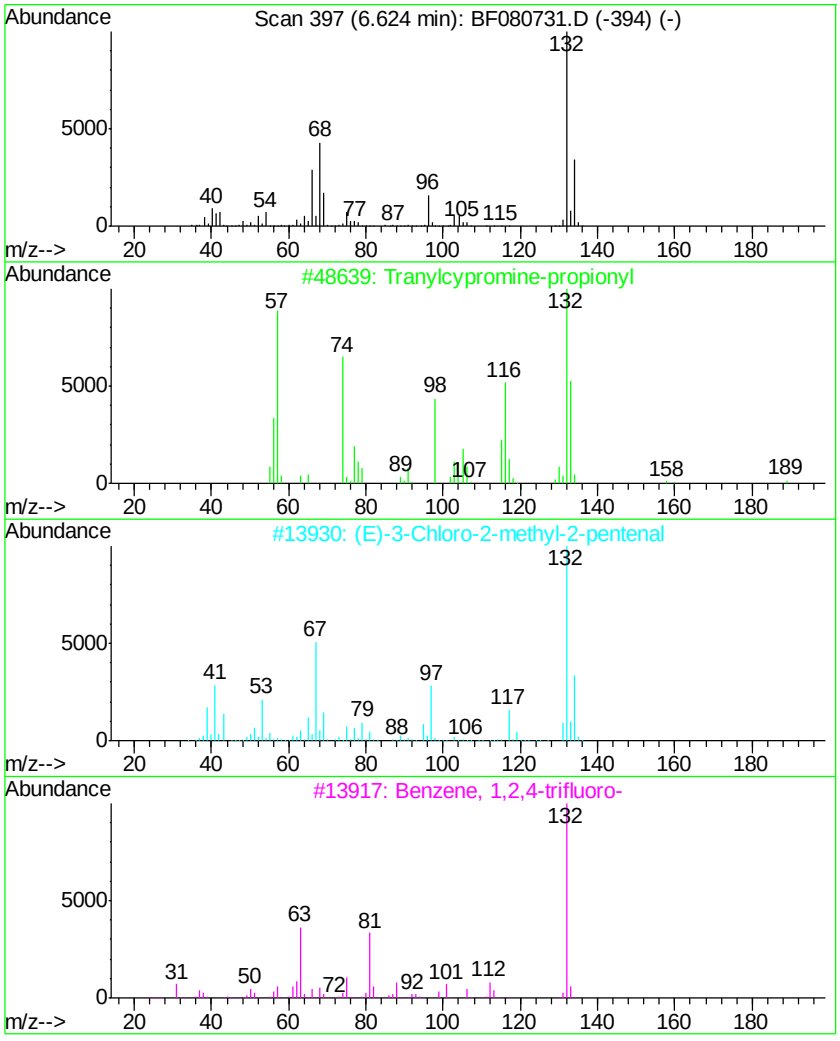
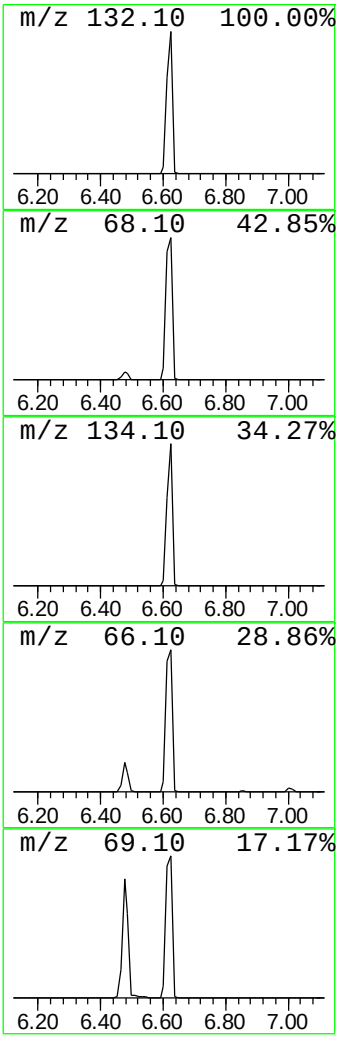
****

Peak Number 5 unknown6.62 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	88.17 ng	4438320	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Xenon	132	Xe	007440-63-3	9





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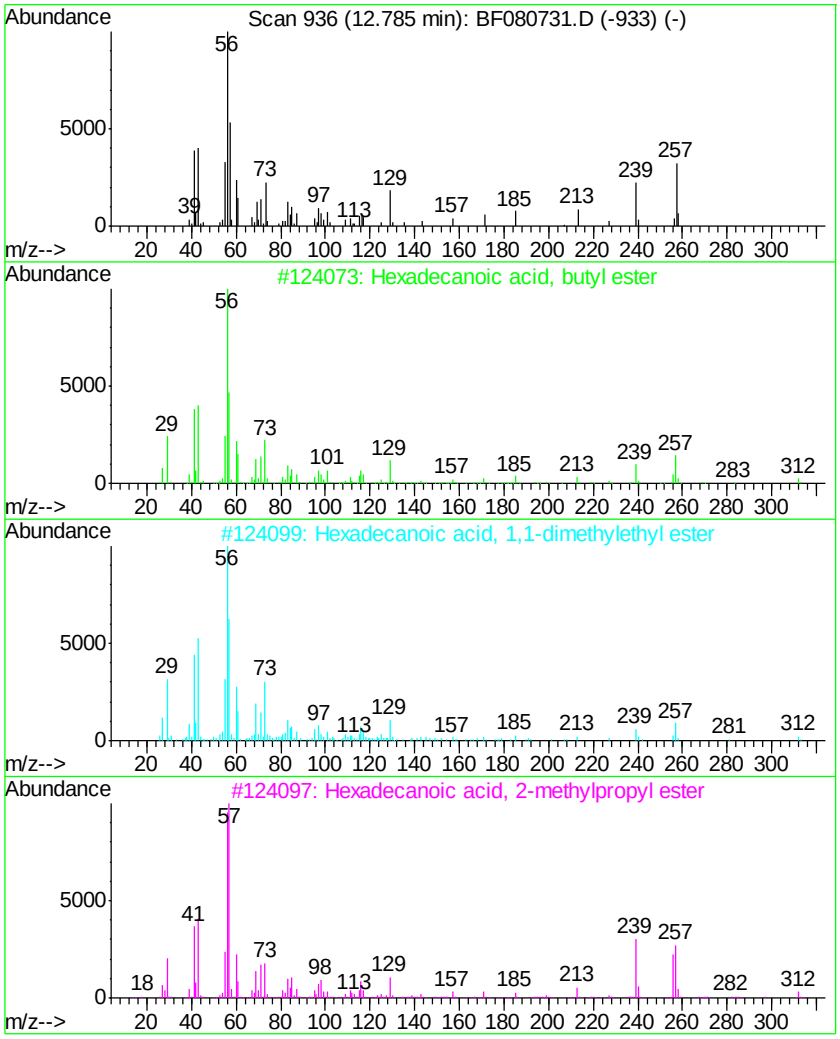
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

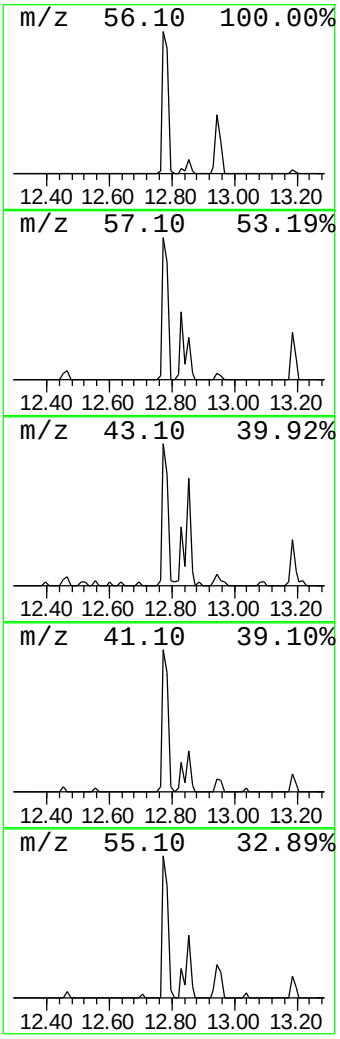
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	4.01 ng	192926	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	38
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

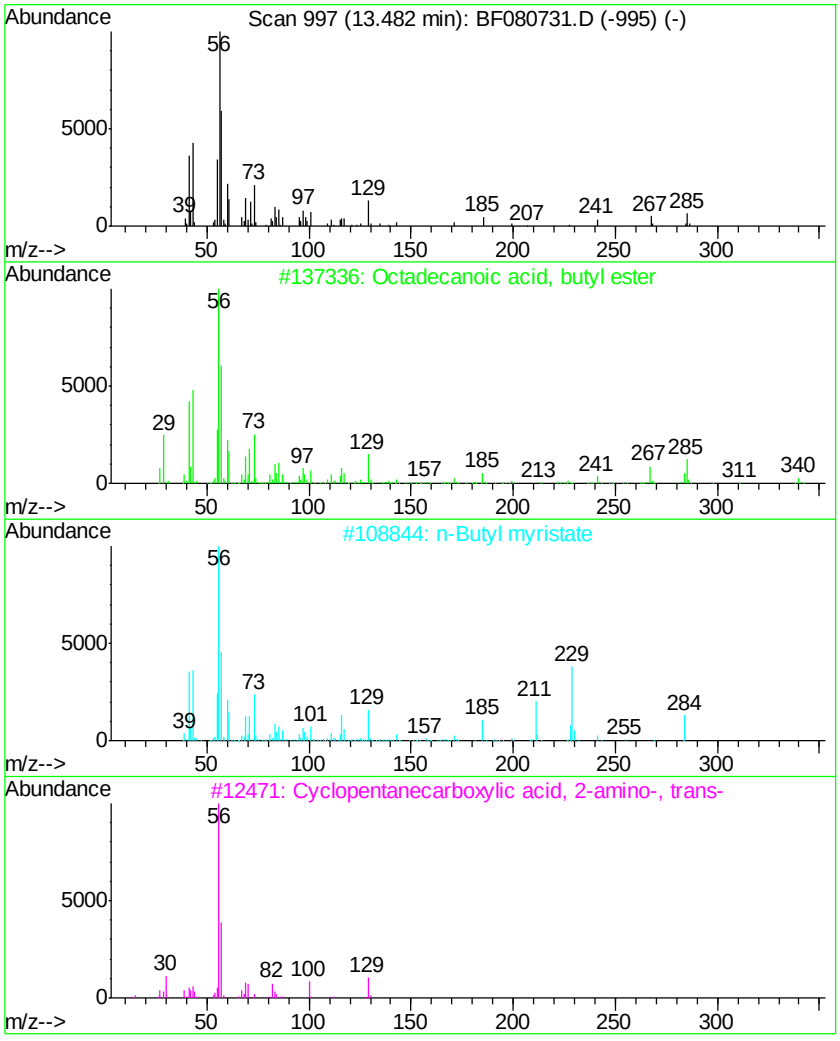
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

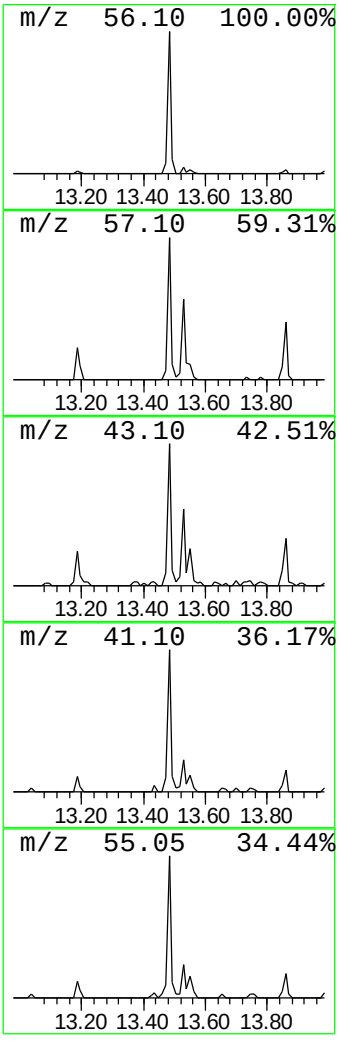
****

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	3.38 ng	162666	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	n-Butyl myristate	284	C18H36O2	000110-36-1	80
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38





Tentatively Identified Compound (LSC) summary

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Operator : TP/UM
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Misc :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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...	3.49	2.1	ng	105737	1	6.85	1006790	20.0
3-Penten-2-one, 4...	4.43	90.5	ng	4553360	1	6.85	1006790	20.0
2-Pentanone, 4-hy...	5.08	143.6	ng	7229700	1	6.85	1006790	20.0
unknown5.87	5.87	7.2	ng	364622	1	6.85	1006790	20.0
unknown6.62	6.62	88.2	ng	4438320	1	6.85	1006790	20.0
Hexadecanoic acid...	12.79	4.0	ng	192926	5	14.00	962353	20.0
Octadecanoic acid...	13.48	3.4	ng	162666	5	14.00	962353	20.0