LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080868.D
Acq On : 5 Aug 2015 7:36
Operator : TP/UM
Sample : G3170-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

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-BF080415.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	2.224	6	12	15	rBV	11065	34253	1.64%	0.229%
2	4.361	196	199	202	rBV	100440	136054	6.51%	0.908%
3	5.013	252	256	258	rBV	527136	754077	36.09%	5.034%
4	5.424	289	292	294	rBV	893756	955490	45.73%	6.378%
5	5.836	325	328	330	rVB	78886	102018	4.88%	0.681%
6	6.442	379	381	384	rBV	505590	509850	24.40%	3.403%
7	6.590	391	394	396	rBV	1593610	1605727	76.85%	10.718%
8	6.750	406	408	412	rBV	19044	23477	1.12%	0.157%
9	6.819	412	414	416	rBV	535019	546154	26.14%	3.646%
10	6.979	425	428	430	rVB	1600221	1448306	69.32%	9.668%
11	7.082	435	437	442	rBB3	15820	30835	1.48%	0.206%
12	7.390	460	464	466	rVB	896184	1320476	63.20%	8.814%
13	7.619	480	484	494	rBB	65436	118793	5.69%	0.793%
14	8.099	524	526	529	rVB	528821	688777	32.96%	4.598%
15	8.693	576	578	580	rVB	35273	39267	1.88%	0.262%
16	9.185	618	621	623	rBV	1960505	2089421	100.00%	13.947%
17	9.573	653	655	657	rVB	32355	24648	1.18%	0.165%
18	9.859	677	680	682	rBV	523731	669941	32.06%	4.472%
19	10.168	705	707	712	rBV	16451	21526	1.03%	0.144%
20	10.339	720	722	724	rBV	45825	42829	2.05%	0.286%
21	10.636	745	748	751	rBV	889911	937137	44.85%	6.256%
22	11.334	806	809	811	rBV	697230	586930	28.09%	3.918%
23	11.871	854	856	858	rBV	21824	26375	1.26%	0.176%
24	12.031	868	870	876	rVB	18238	22666	1.08%	0.151%
25	12.922	945	948	950	rBV	1229232	1333278	63.81%	8.900%
26	13.482	995	997	1001	rVB	318220	275077	13.17%	1.836%
27	13.962	1036	1039	1041	rBV	373211	378640	18.12%	2.527%
28	15.368	1159	1162	1165	rBV	224860	258973	12.39%	1.729%

Sum of corrected areas: 14980995

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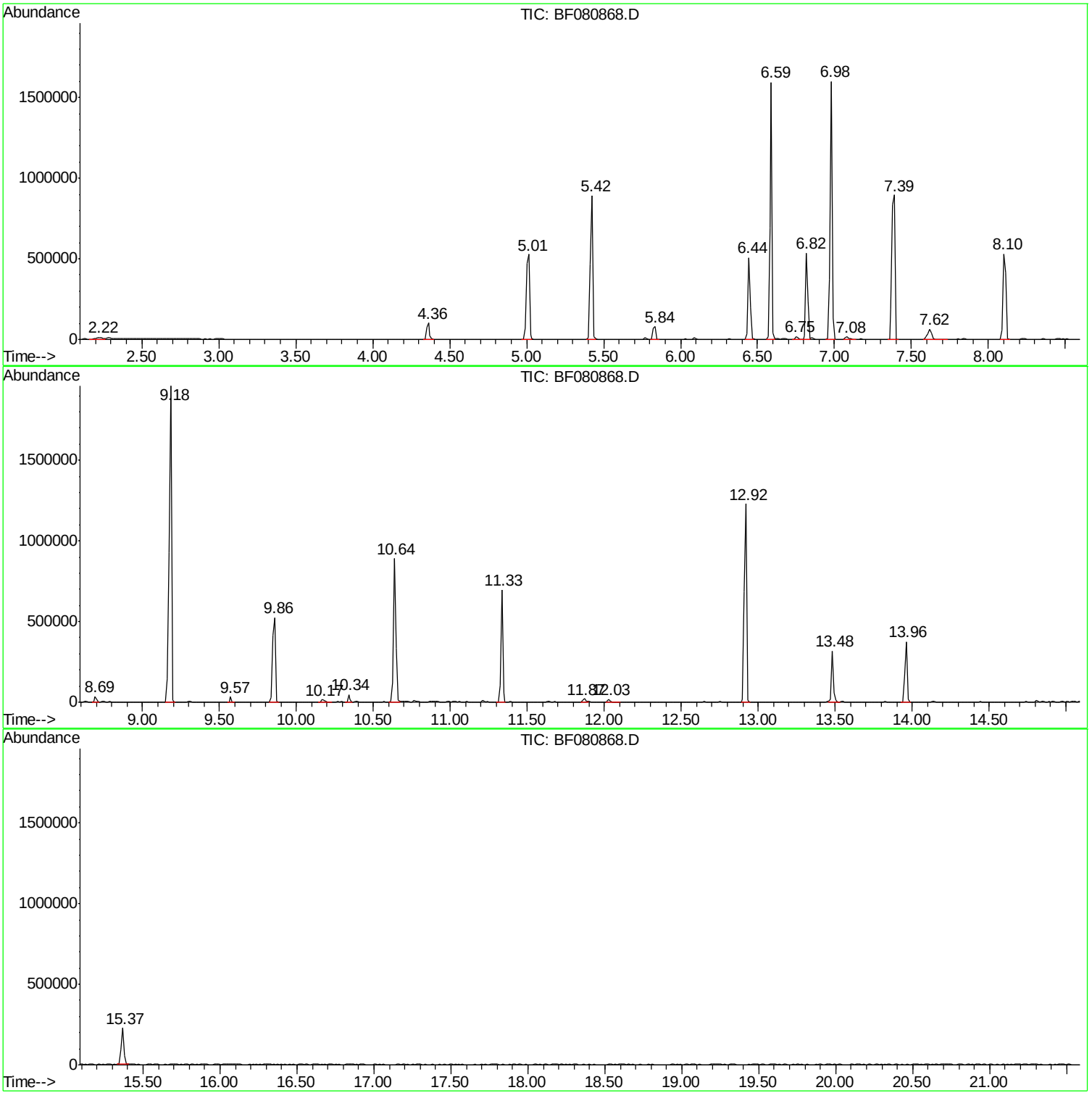
Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.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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Acq On : 5 Aug 2015 7:36
Operator : TP/UM
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

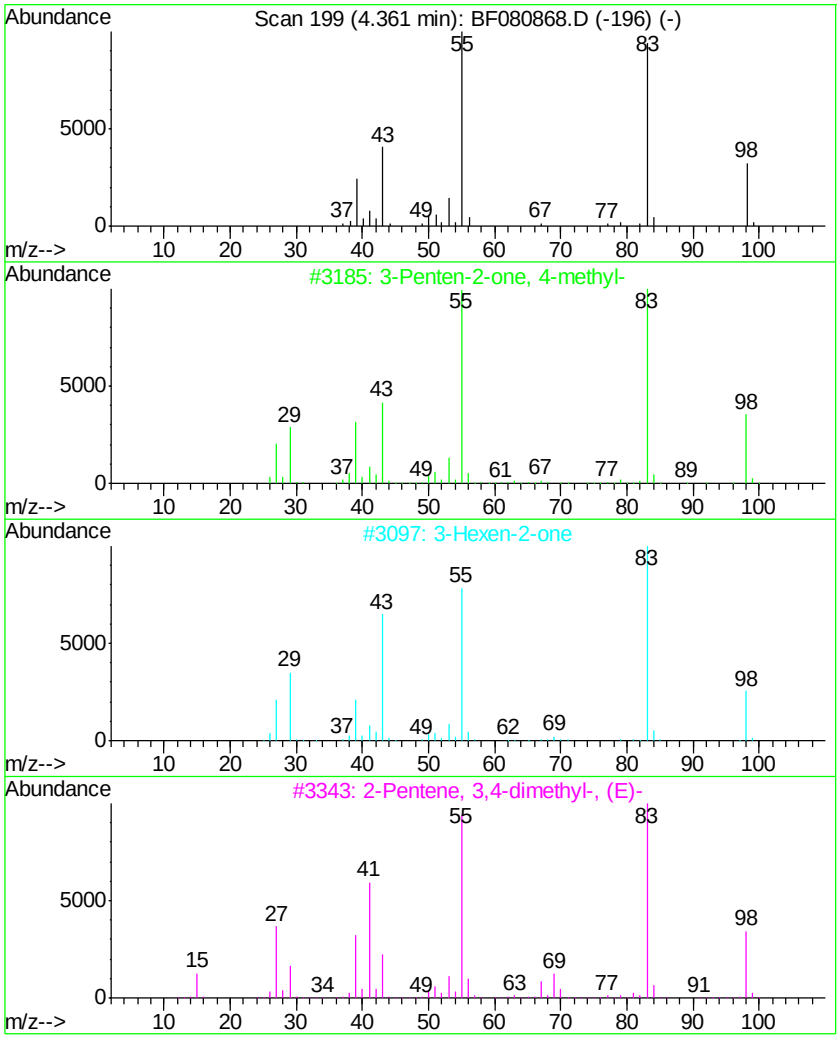
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

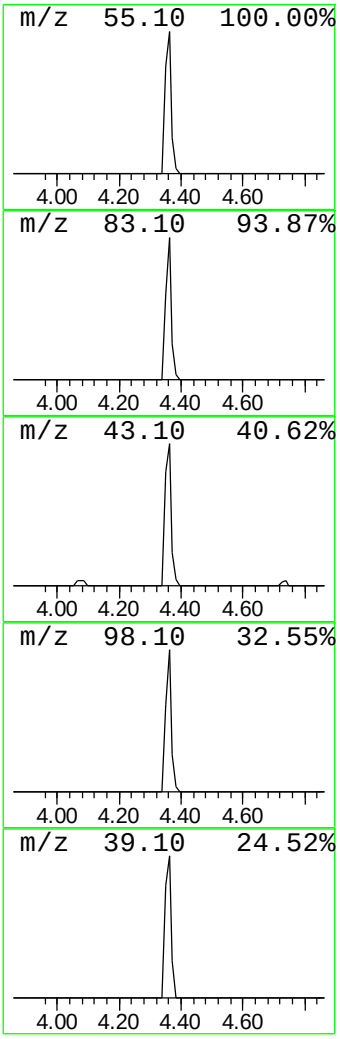
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	4.98 ng	136054	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, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Operator : TP/UM
Sample : G3170-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.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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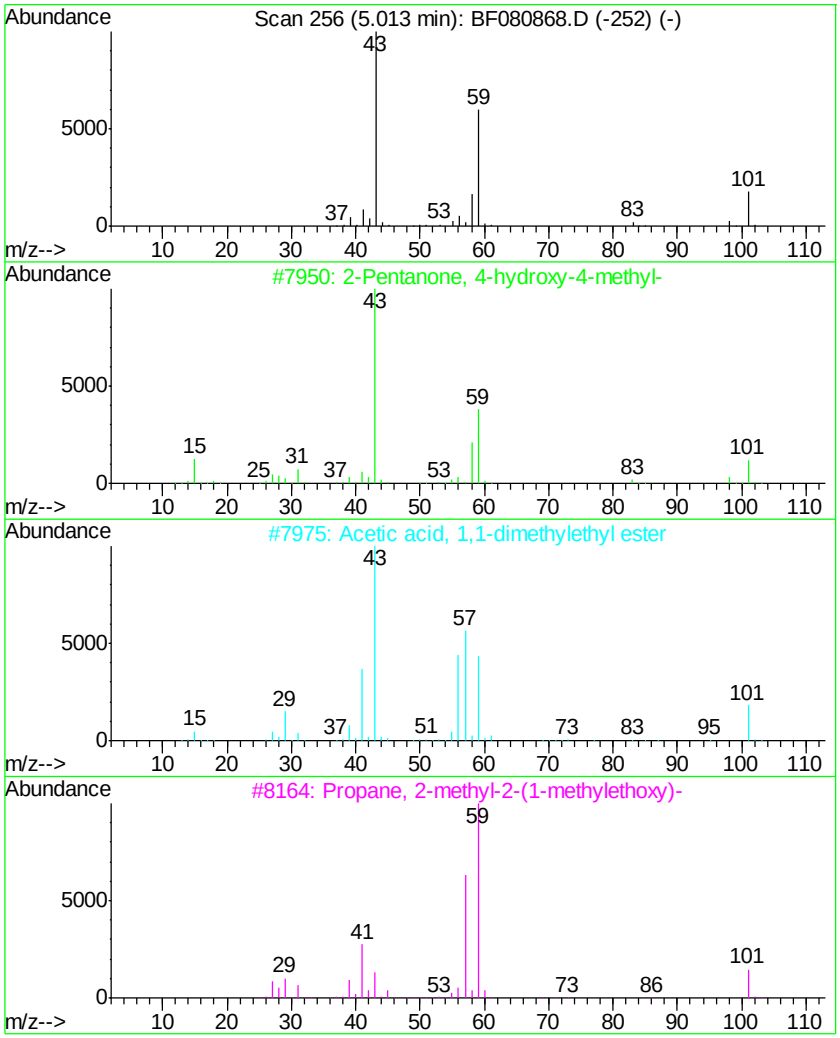
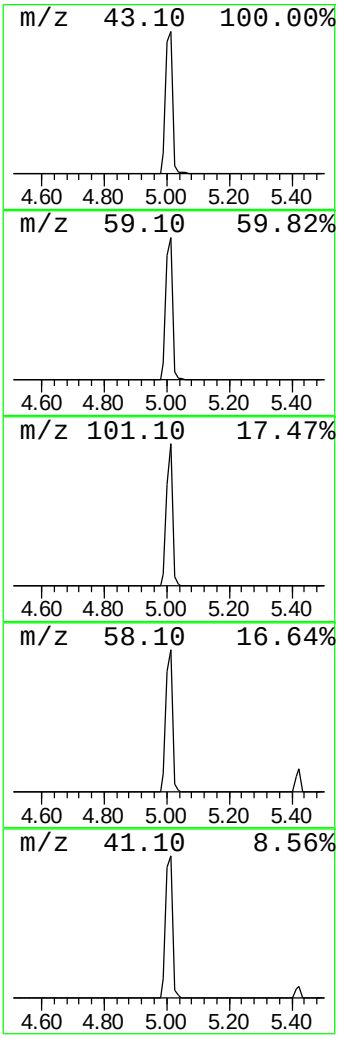
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	27.61 ng	754077	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080868.D
Acq On : 5 Aug 2015 7:36
Operator : TP/UM
Sample : G3170-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.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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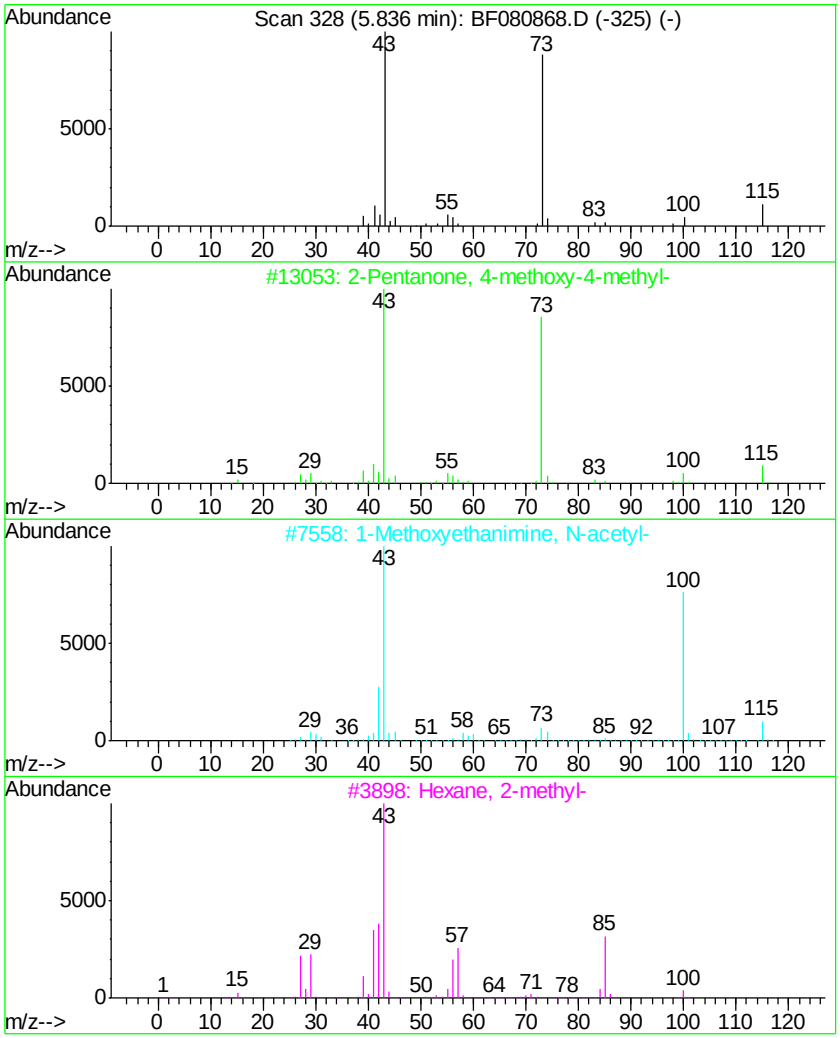
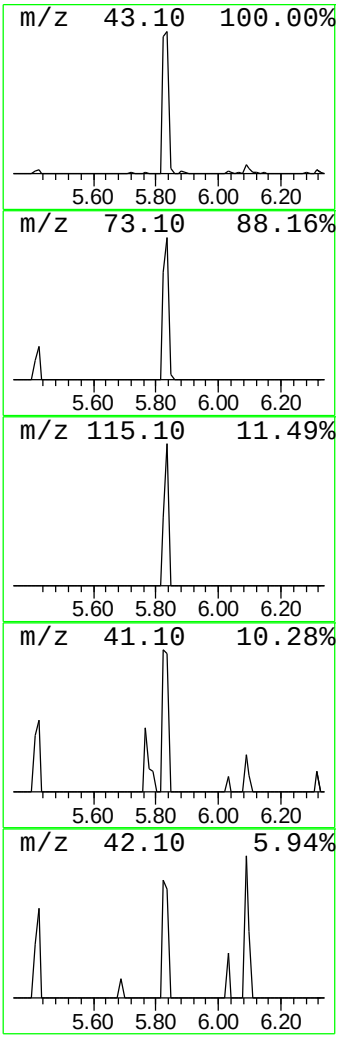
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.84	3.74 ng	102018	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	90
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	37
3	Hexane, 2-methyl-	100	C7H16	000591-76-4	9
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





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Operator : TP/UM
Sample : G3170-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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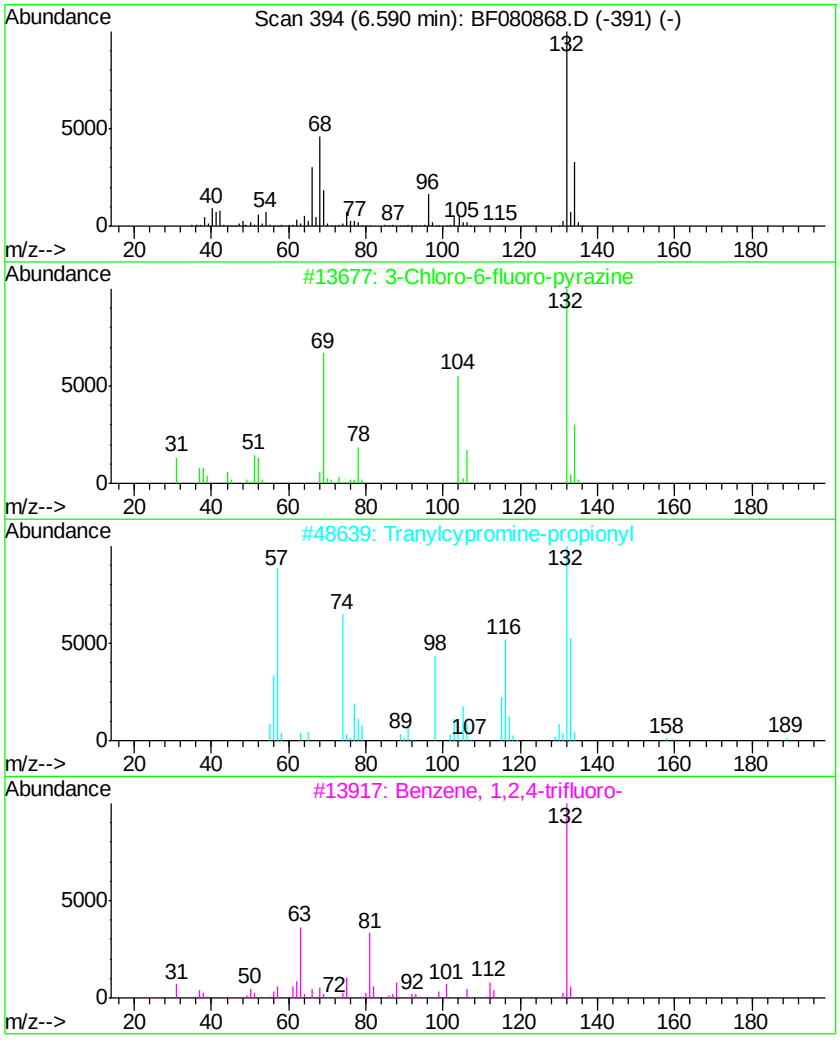
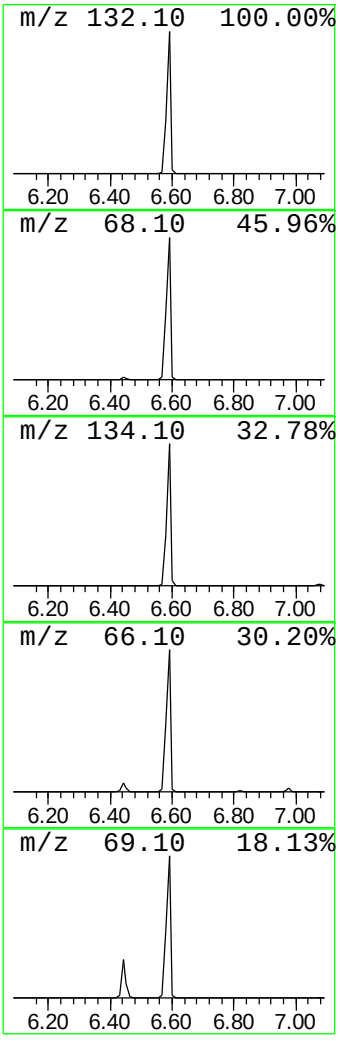
Peak Number 4 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	58.80 ng	1605730	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Sample : G3170-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.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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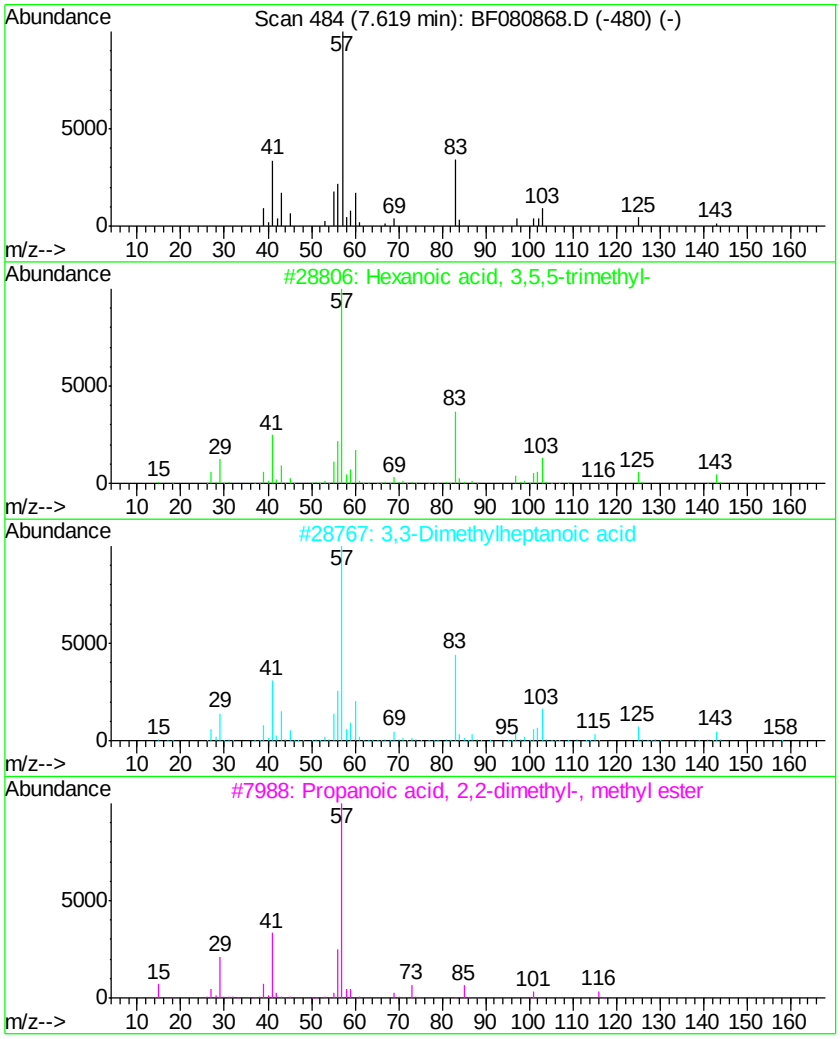
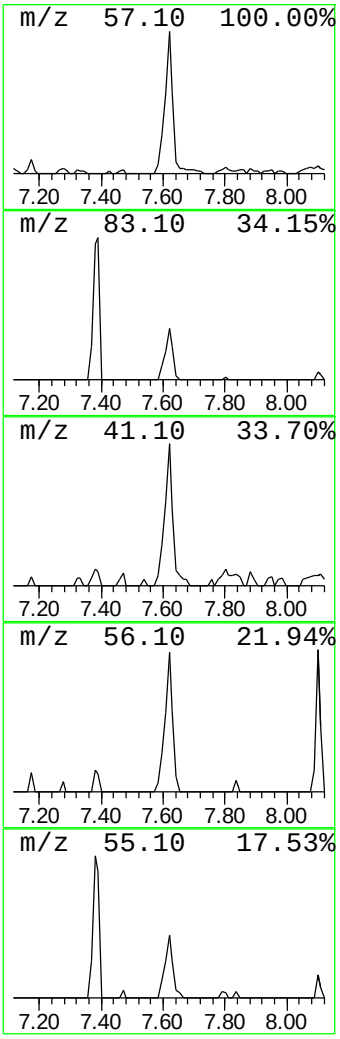
Peak Number 6 Hexanoic acid, 3,5,5-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	3.45 ng	118793	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	83
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3	Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	38
4	Carbonic acid, bis(1-methylpropy...	174	C9H18O3	000623-63-2	23
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12





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ClientSampleId : MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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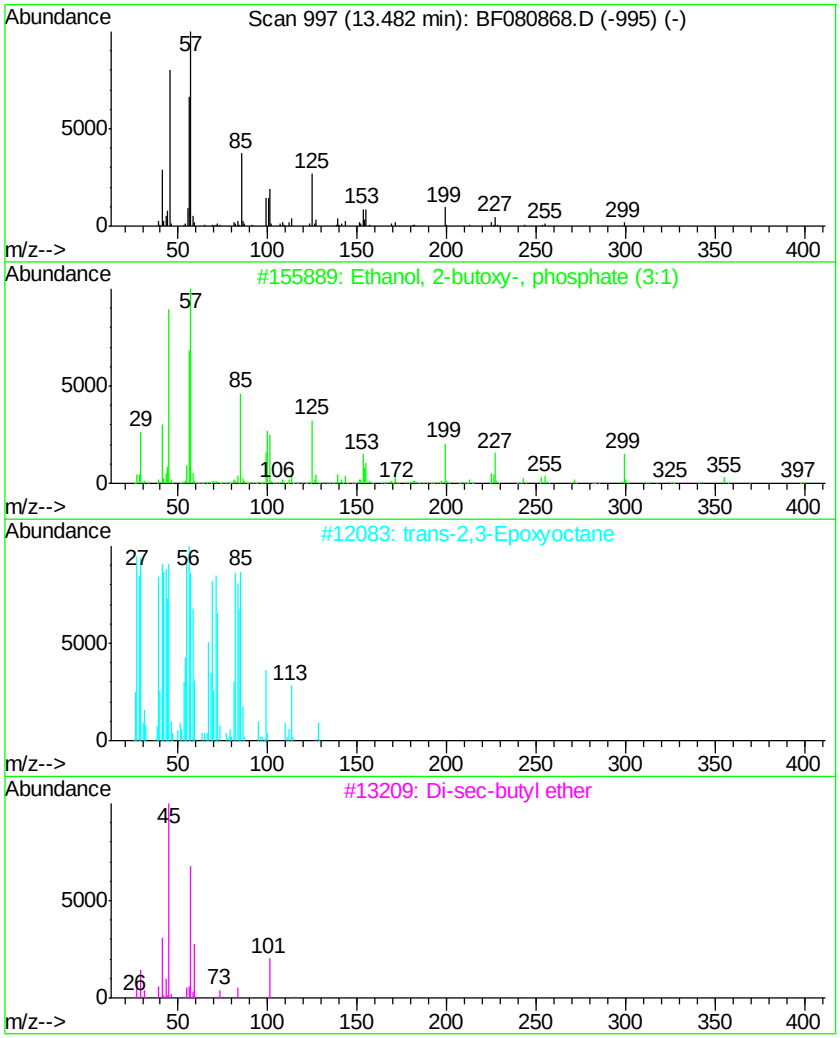
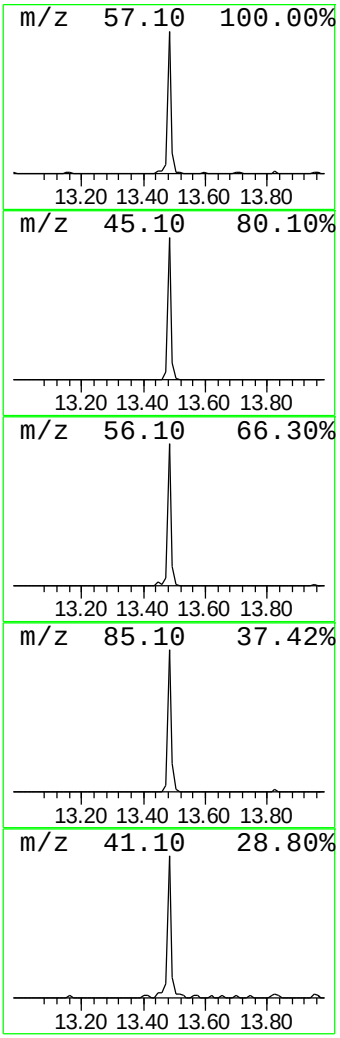
Peak Number 7 Ethanol, 2-butoxy-, phospha... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	14.53 ng	275077	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	86
2	trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	47
3	Di-sec-butyl ether	130	C8H18O	006863-58-7	38
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	38
5	2,5-Hexanediol	118	C6H14O2	002935-44-6	38





Tentatively Identified Compound (LSC) summary

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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...	4.36	5.0	ng	136054	1	6.82	546154	20.0
2-Pentanone, 4-hy...	5.01	27.6	ng	754077	1	6.82	546154	20.0
2-Pentanone, 4-me...	5.84	3.7	ng	102018	1	6.82	546154	20.0
unknown6.59	6.59	58.8	ng	1605730	1	6.82	546154	20.0
Hexanoic acid, 3,...	7.62	3.5	ng	118793	2	8.10	688777	20.0
Ethanol, 2-butoxy...	13.48	14.5	ng	275077	5	13.96	378640	20.0