LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080866.D
Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-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-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	7	12	16	rBV	7665	27592	1.23%	0.154%
2	4.361	196	199	202	rVB	87752	132199	5.91%	0.737%
3	5.001	252	255	258	rBV	487659	676454	30.27%	3.770%
4	5.424	289	292	294	rBV	693889	867911	38.83%	4.837%
5	5.836	326	328	330	rBV	79454	98678	4.41%	0.550%
6	6.442	379	381	384	rBV	469580	482163	21.57%	2.687%
7	6.590	391	394	396	rBV	1614873	1584260	70.88%	8.829%
8	6.750	407	408	412	rBV	35634	48607	2.17%	0.271%
9	6.819	412	414	416	rVV	536931	573989	25.68%	3.199%
10	6.853	416	417	420	rVB	33483	30442	1.36%	0.170%
11	6.979	425	428	430	rVB	1554858	1379995	61.74%	7.690%
12	7.047	430	434	438	rBV	95844	154282	6.90%	0.860%
13	7.390	460	464	466	rVB	1071540	1388514	62.12%	7.738%
14	7.642	480	486	488	rBV	165548	311045	13.92%	1.733%
15	8.099	524	526	529	rVB	527848	734495	32.86%	4.093%
16	8.225	535	537	540	rBV	20464	24217	1.08%	0.135%
17	8.362	545	549	551	rBV	15187	22770	1.02%	0.127%
18	8.465	553	558	560	rBV	20671	38296	1.71%	0.213%
19	8.693	570	578	580	rVB2	26948	59586	2.67%	0.332%
20	9.185	618	621	623	rBV	2127619	2235066	100.00%	12.455%
21	9.573	653	655	657	rVB	70456	54269	2.43%	0.302%
22	9.859	677	680	682	rBV	638017	747126	33.43%	4.163%
23	10.168	705	707	712	rBV	35397	49561	2.22%	0.276%
24	10.396	724	727	730	rVB	34591	36964	1.65%	0.206%
25	10.636	745	748	751	rBV	982433	1073086	48.01%	5.980%
26	10.762	758	759	764	rVB	16922	24160	1.08%	0.135%
27	11.333	806	809	811	rBV	803202	676745	30.28%	3.771%
28	11.871	853	856	858	rBV	48938	57441	2.57%	0.320%
29	12.031	868	870	874	rVB	40896	43818	1.96%	0.244%
30	12.614	916	921	923	rBV2	35340	38667	1.73%	0.215%
31	12.922	945	948	950	rBV	1420062	1459452	65.30%	8.133%
32	13.482	995	997	1000	rVB	1480001	1986134	88.86%	11.068%
33	13.962	1036	1039	1041	rBV	447204	438970	19.64%	2.446%
34	14.808	1111	1113	1116	rVB	105140	101326	4.53%	0.565%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080866.D
Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-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-BF080415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.368	1159	1162	1165	rBV	248265	286550	12.82%	1.597%

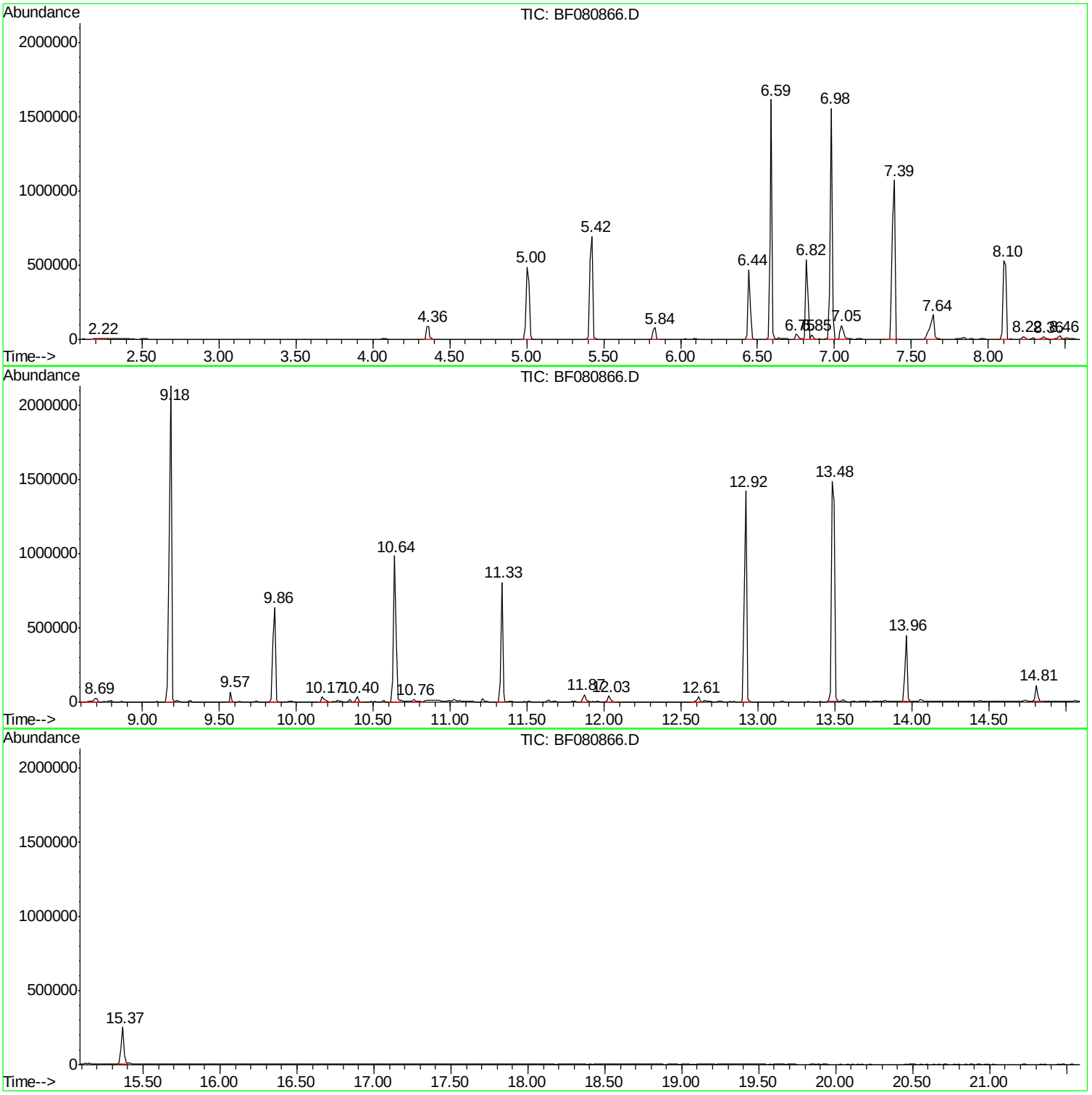
Sum of corrected areas: 17944830

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080866.D
Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080866.D
Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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

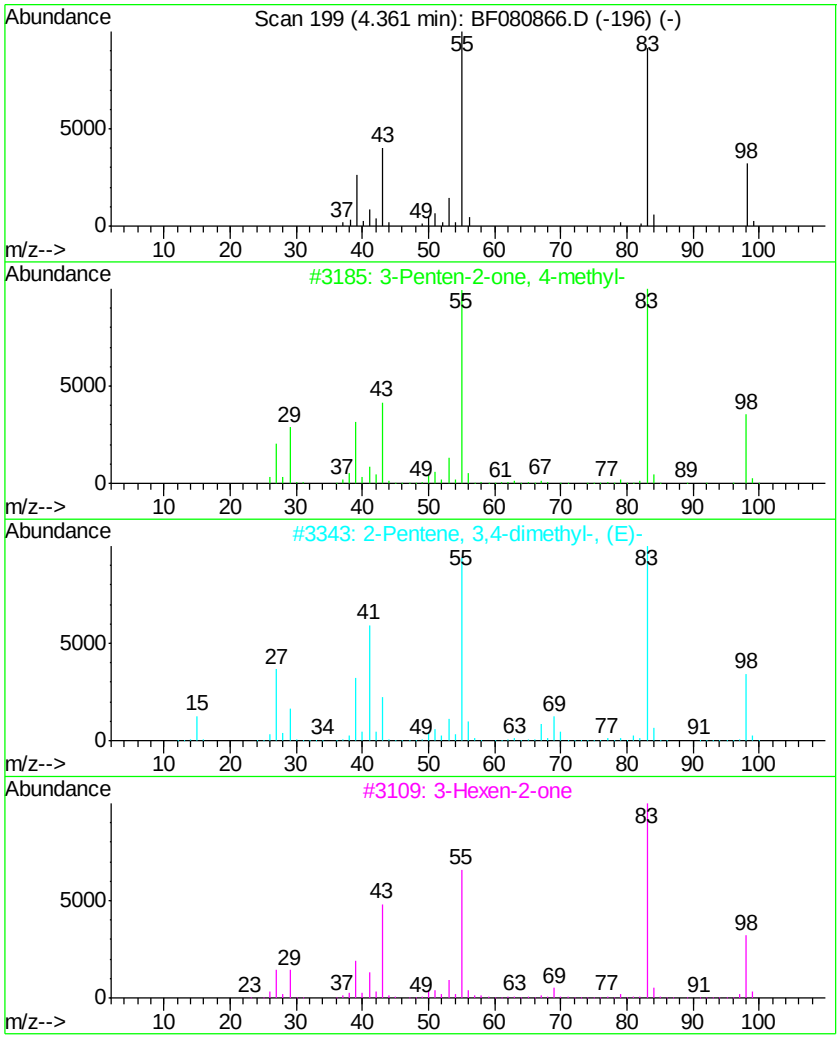
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

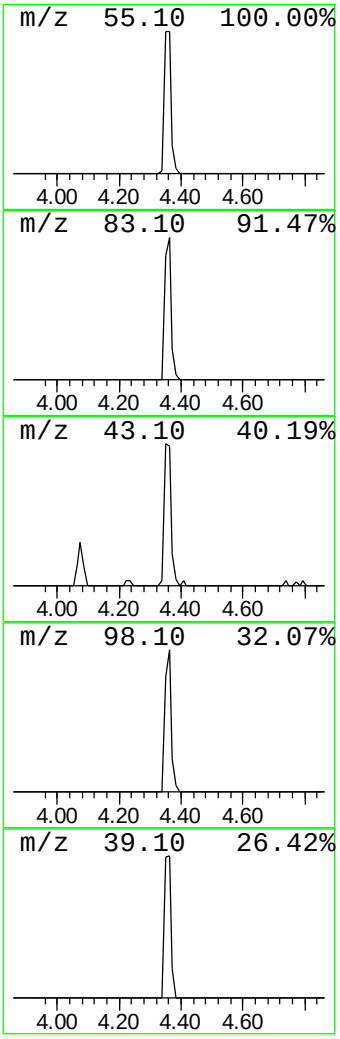
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	4.61 ng	132199	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	94
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	87
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080866.D
Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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

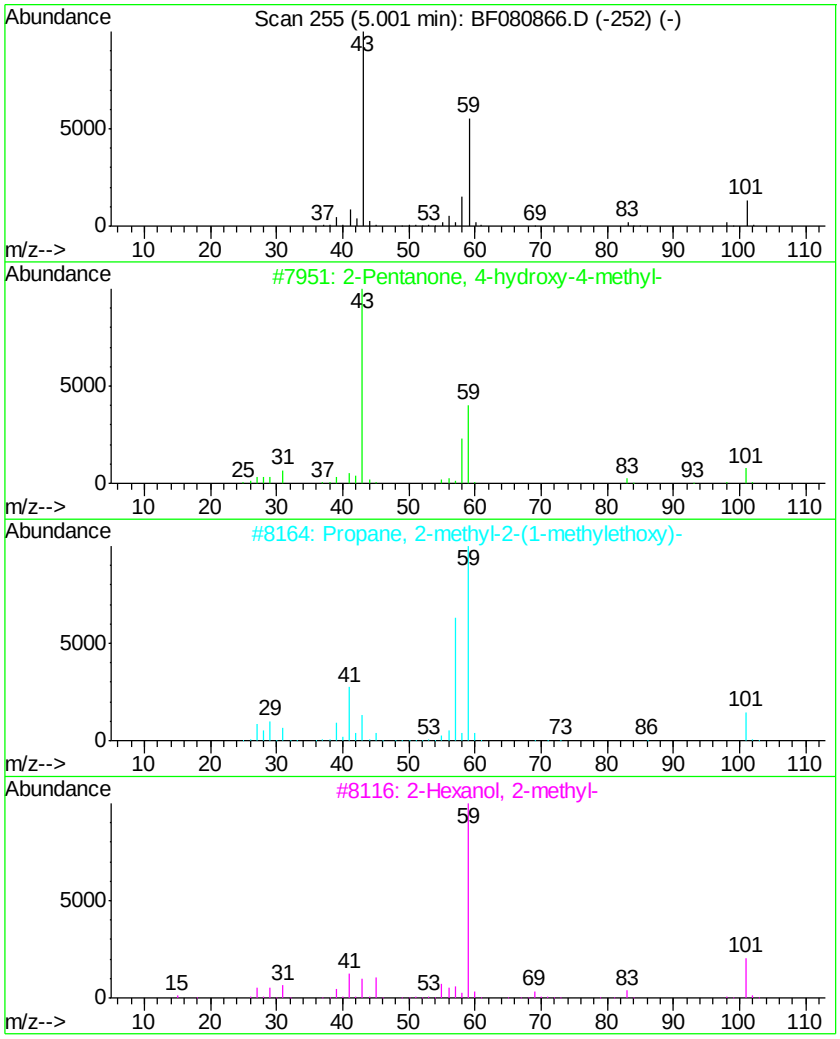
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

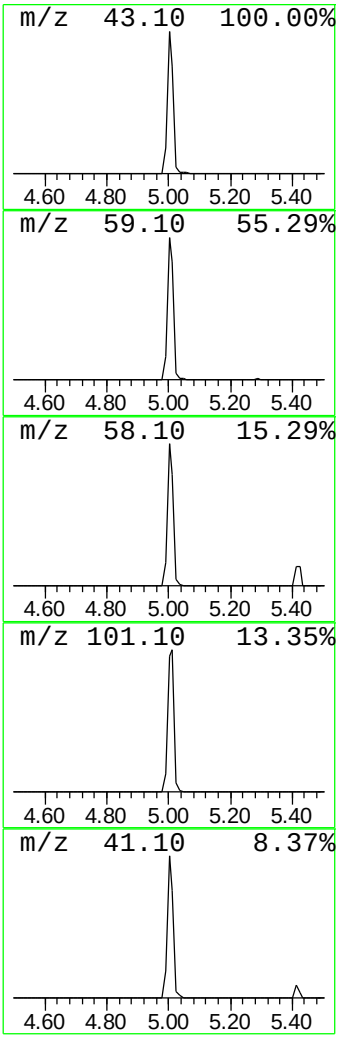
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	23.57 ng	676454	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	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080866.D
Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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

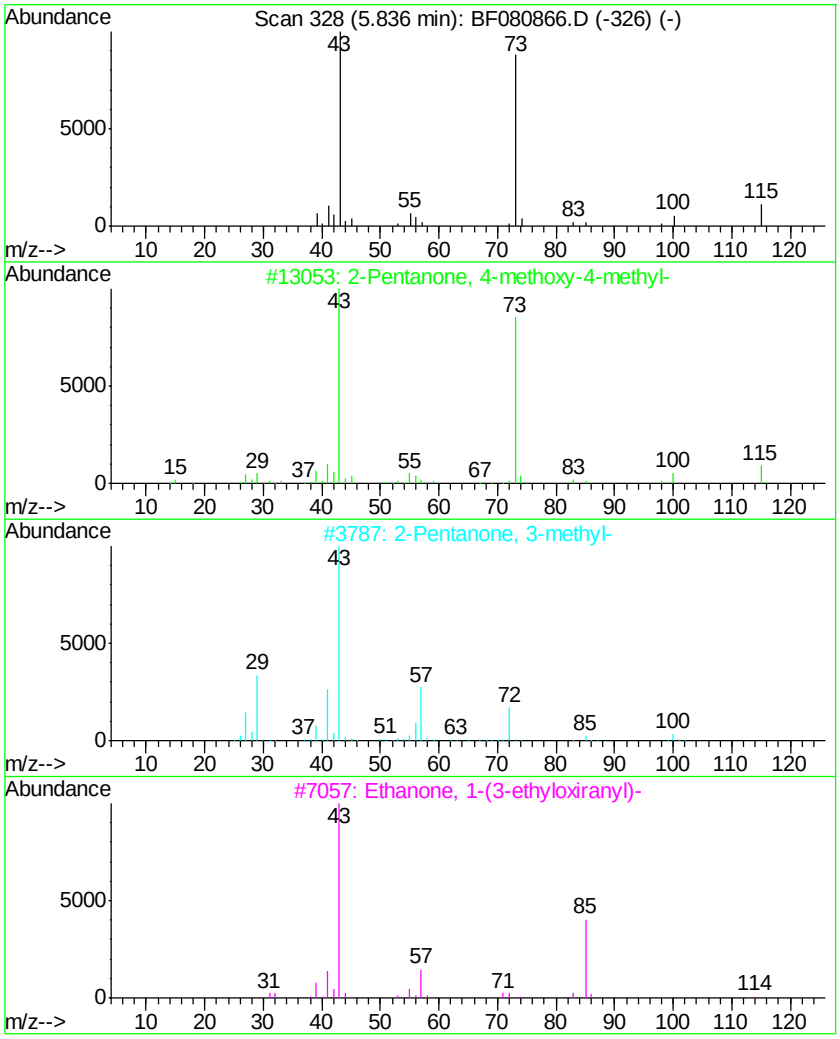
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

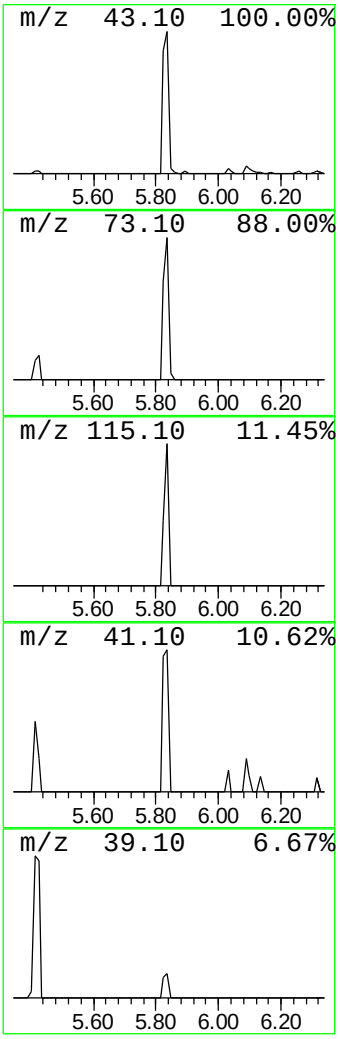
****

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.84	3.44 ng	98678	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	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
3	Ethanone, 1-(3-ethyloxiranyl)-	114	C6H10O2	017257-81-7	10
4	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
5	Hexane, 2-methyl-	100	C7H16	000591-76-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080866.D
Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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

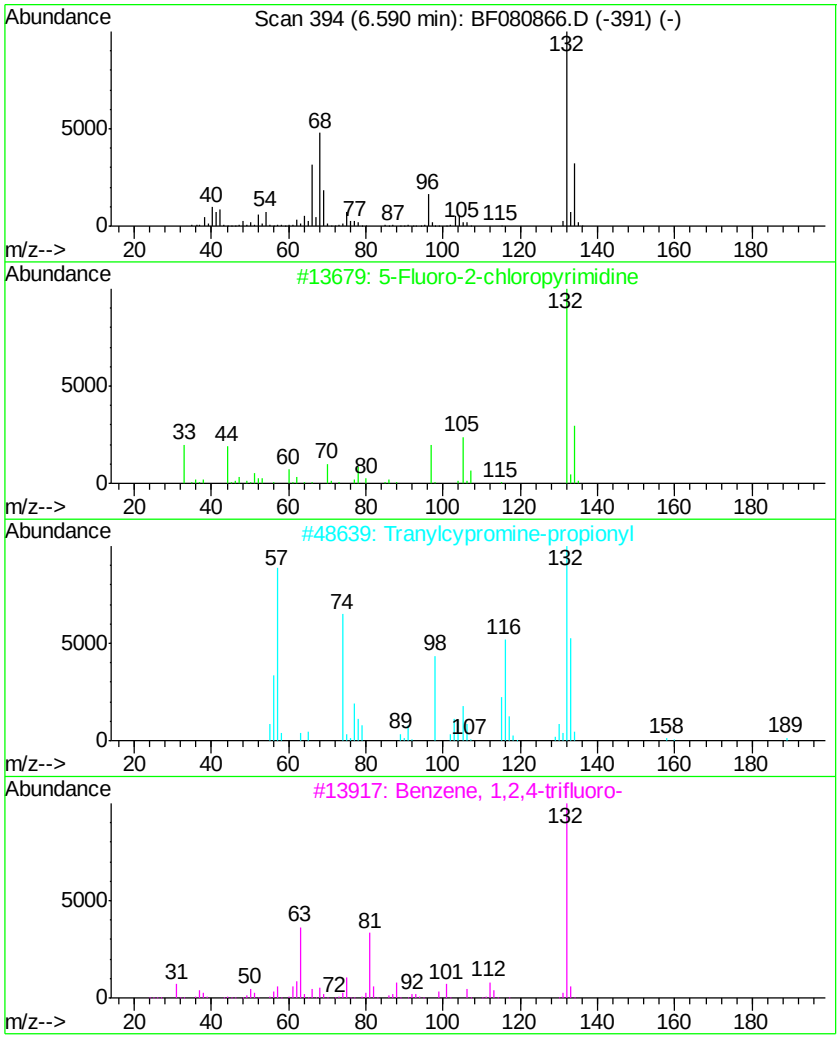
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

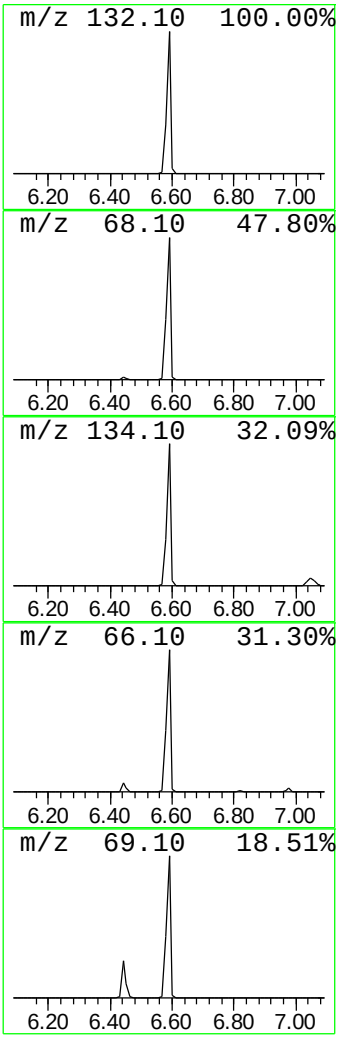
****

Peak Number 4 unknown6.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	55.20 ng	1584260	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
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	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080866.D
Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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

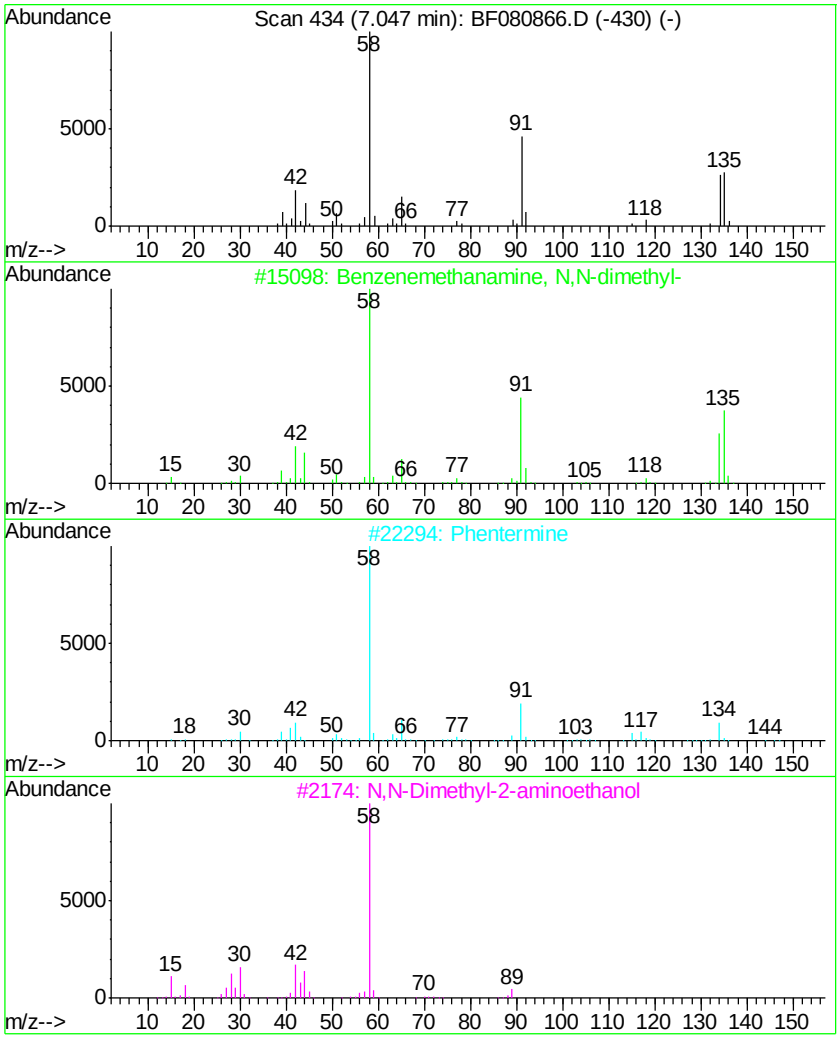
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

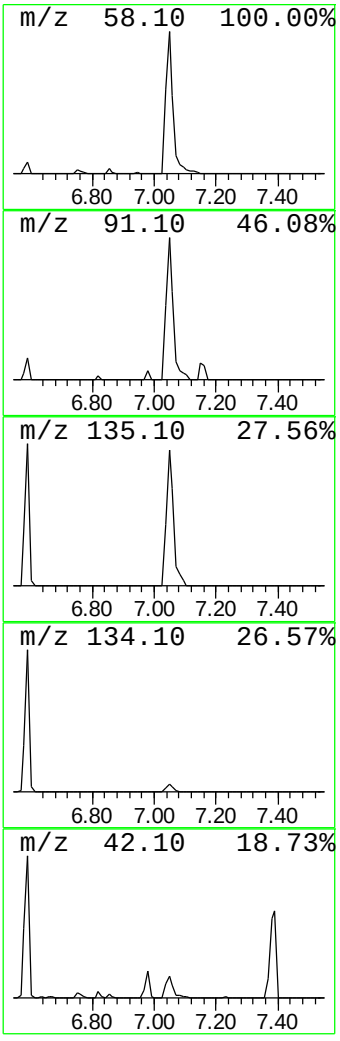
****

Peak Number 6 Benzenemethanamine, N,N-dim... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	5.38 ng	154282	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanamine, N,N-dimethyl-	135	C9H13N	000103-83-3	95
2	Phentermine	149	C10H15N	000122-09-8	64
3	N,N-Dimethyl-2-aminoethanol	89	C4H11NO	000108-01-0	47
4	Cetalkonium Chloride	395	C25H46ClN	000122-18-9	42
5	Carbachol	182	C6H15ClN2O2	000051-83-2	38





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Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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

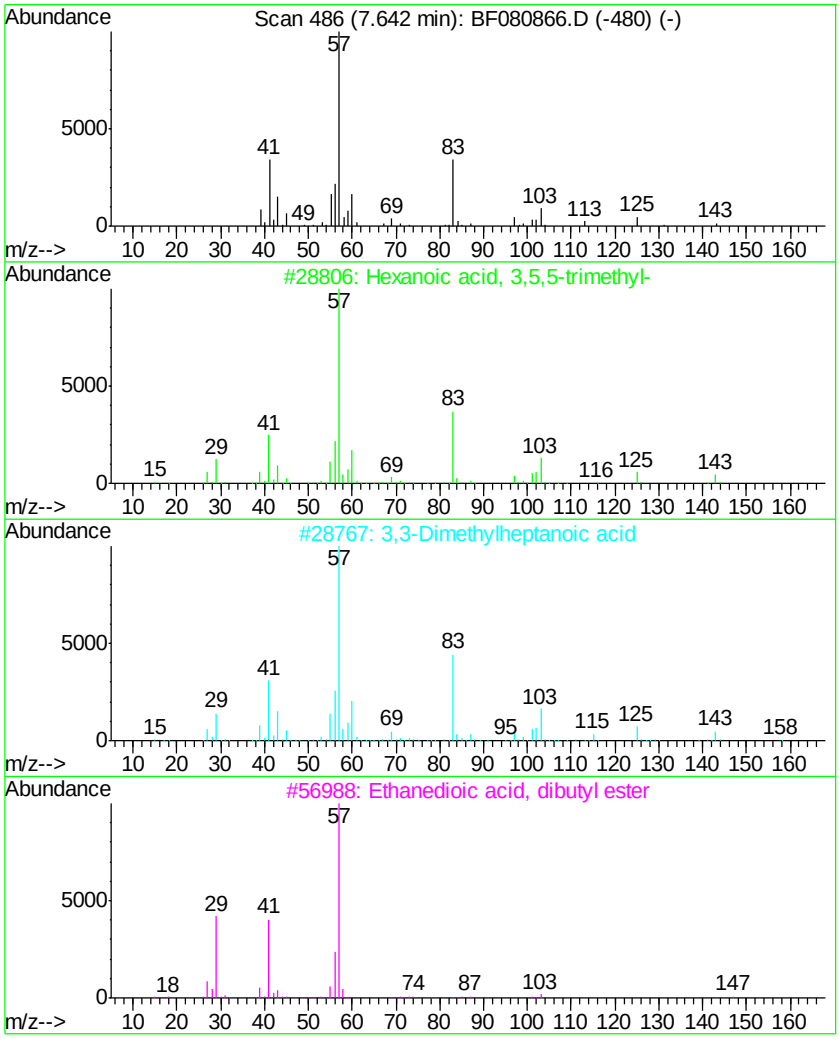
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

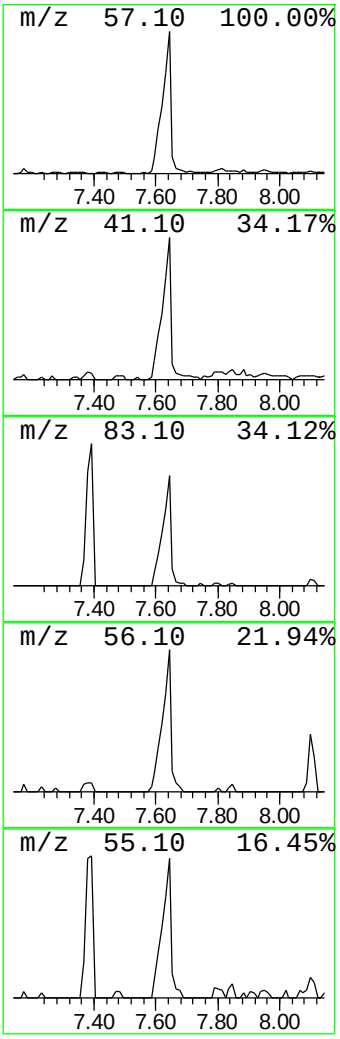
****

Peak Number 7 Hexanoic acid, 3,5,5-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	8.47 ng	311045	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	83
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3	Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	27
4	Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	25
5	Pivalic acid, 2-methylpropyl ester	158	C9H18O2	005129-38-4	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
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Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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

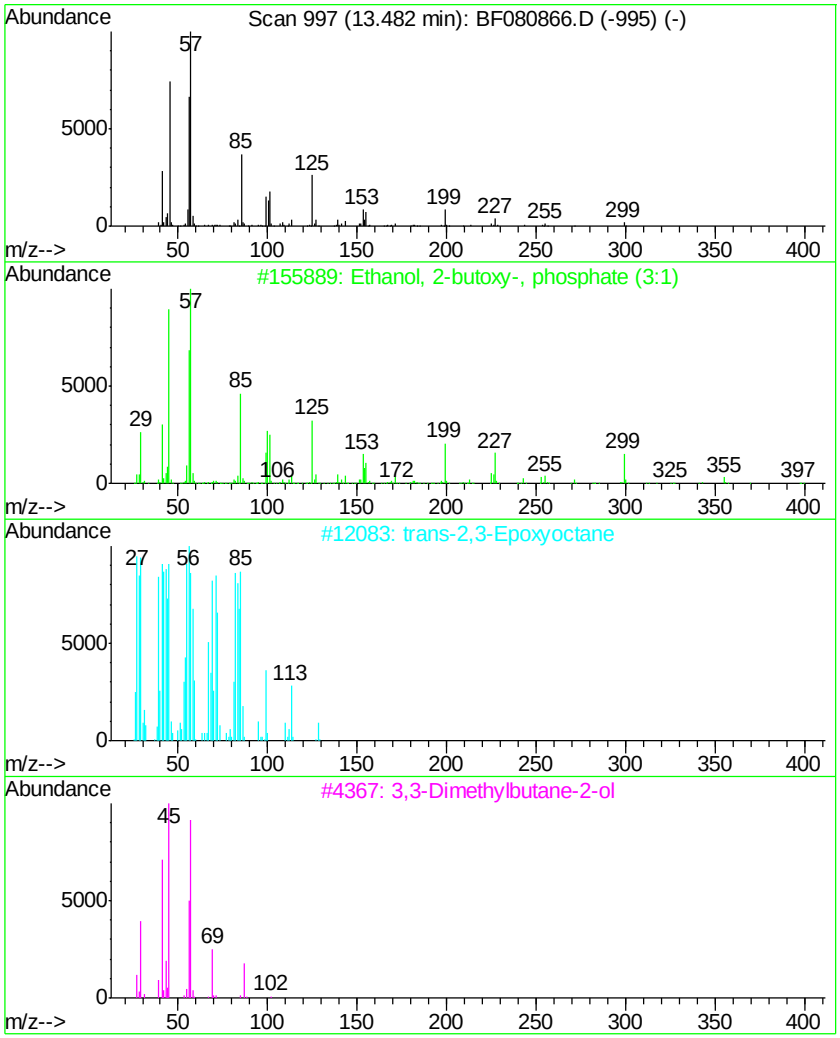
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

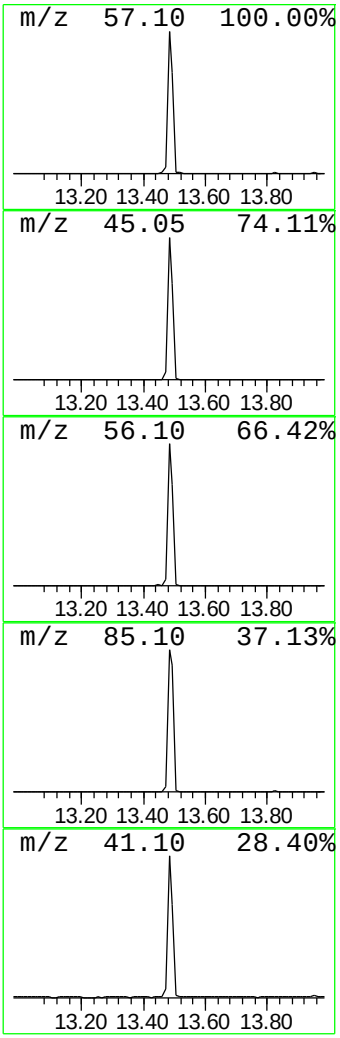
****

Peak Number 8 Ethanol, 2-butoxy-, phospha... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	90.49 ng	1986130	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	72
2	trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	47
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	43
4	2,5-Hexanediol	118	C6H14O2	002935-44-6	40
5	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	40





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080866.D
Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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

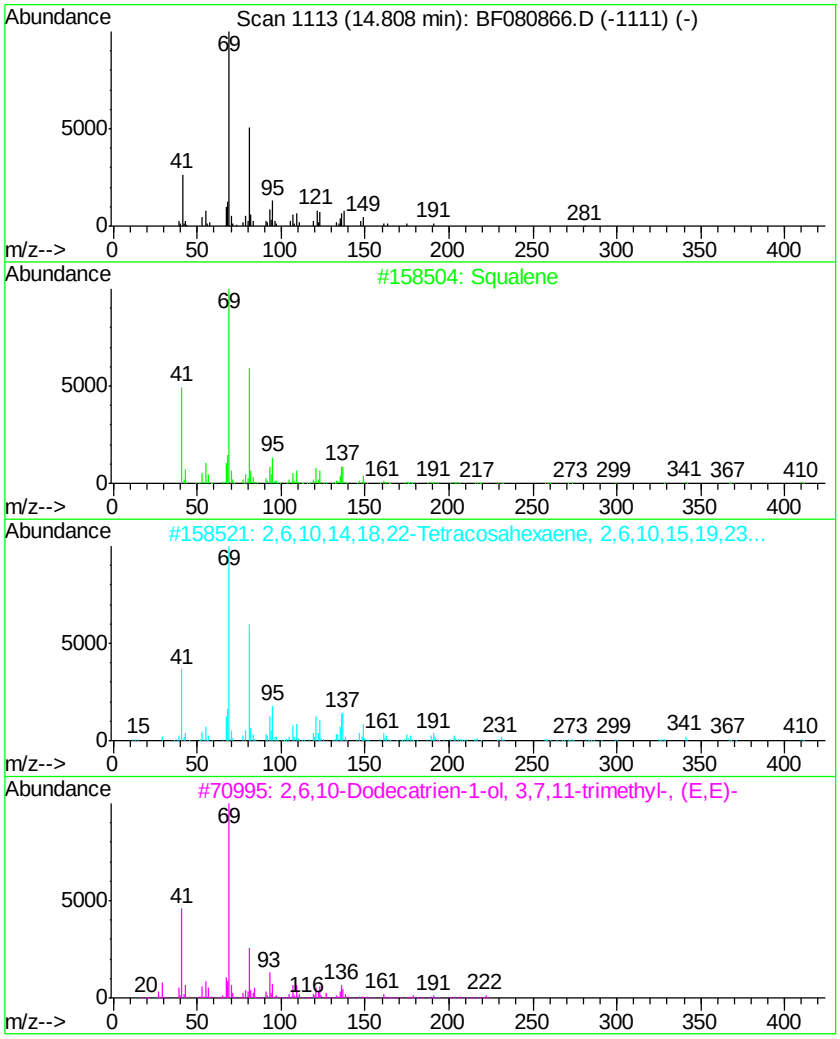
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

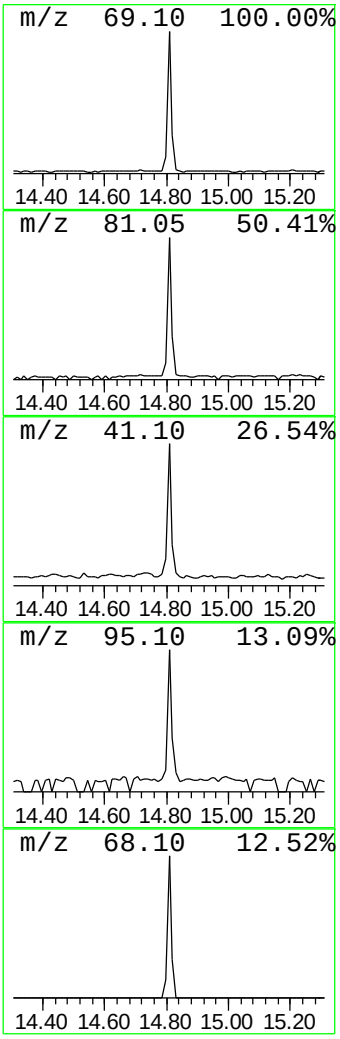
****

Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	7.07 ng	101326	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	83
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
Data File : BF080866.D
Acq On : 5 Aug 2015 6:35
Operator : TP/UM
Sample : G3170-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-2

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.36	4.6	ng	132199	1	6.82	573989	20.0
2-Pentanone, 4-hy...	5.00	23.6	ng	676454	1	6.82	573989	20.0
2-Pentanone, 4-me...	5.84	3.4	ng	98678	1	6.82	573989	20.0
unknown6.59	6.59	55.2	ng	1584260	1	6.82	573989	20.0
Benzenemethanamin...	7.05	5.4	ng	154282	1	6.82	573989	20.0
Hexanoic acid, 3,...	7.64	8.5	ng	311045	2	8.11	734495	20.0
Ethanol, 2-butoxy...	13.48	90.5	ng	1986130	5	13.96	438970	20.0
Squalene	14.81	7.1	ng	101326	6	15.37	286550	20.0