LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101076.D
Acq On : 1 Dec 2017 21:05
Operator : SJ/JU
Sample : I6622-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBWW1B-4-9

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-BF113017.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	5.081	505	509	519	rBV	50830	81217	3.96%	0.656%
2	5.486	573	578	592	rBB	1289952	1397713	68.13%	11.289%
3	5.804	623	632	643	rBV2	21170	35848	1.75%	0.290%
4	6.504	743	751	755	rBV	1146634	2051468	100.00%	16.569%
5	6.628	767	772	775	rBV	1538816	1441759	70.28%	11.645%
6	6.845	806	809	813	rVB	356080	288363	14.06%	2.329%
7	7.004	832	836	839	rBV	1267726	1099433	53.59%	8.880%
8	7.416	901	906	909	rBV	925147	850542	41.46%	6.870%
9	8.127	1023	1027	1031	rBV	454707	370013	18.04%	2.988%
10	8.286	1051	1054	1069	rBV	27174	42778	2.09%	0.346%
11	9.204	1206	1210	1213	rBV	1704382	1566137	76.34%	12.649%
12	9.598	1273	1277	1279	rBV	89004	71038	3.46%	0.574%
13	9.804	1309	1312	1315	rVB	30467	21648	1.06%	0.175%
14	9.886	1322	1326	1329	rBV	447285	367343	17.91%	2.967%
15	10.304	1394	1397	1400	rVB	30193	21934	1.07%	0.177%
16	10.674	1456	1460	1463	rBV	774293	660017	32.17%	5.331%
17	10.780	1474	1478	1486	rVB	18490	21740	1.06%	0.176%
18	11.374	1575	1579	1582	rBV	337588	298092	14.53%	2.408%
19	12.957	1844	1848	1851	rBV	1217799	1040329	50.71%	8.402%
20	13.839	1995	1998	2005	rBV	77042	83324	4.06%	0.673%
21	14.015	2024	2028	2031	rBV	364626	304689	14.85%	2.461%
22	15.486	2273	2278	2283	rBV	227467	265823	12.96%	2.147%

Sum of corrected areas: 12381248

LSC Report - Integrated Chromatogram

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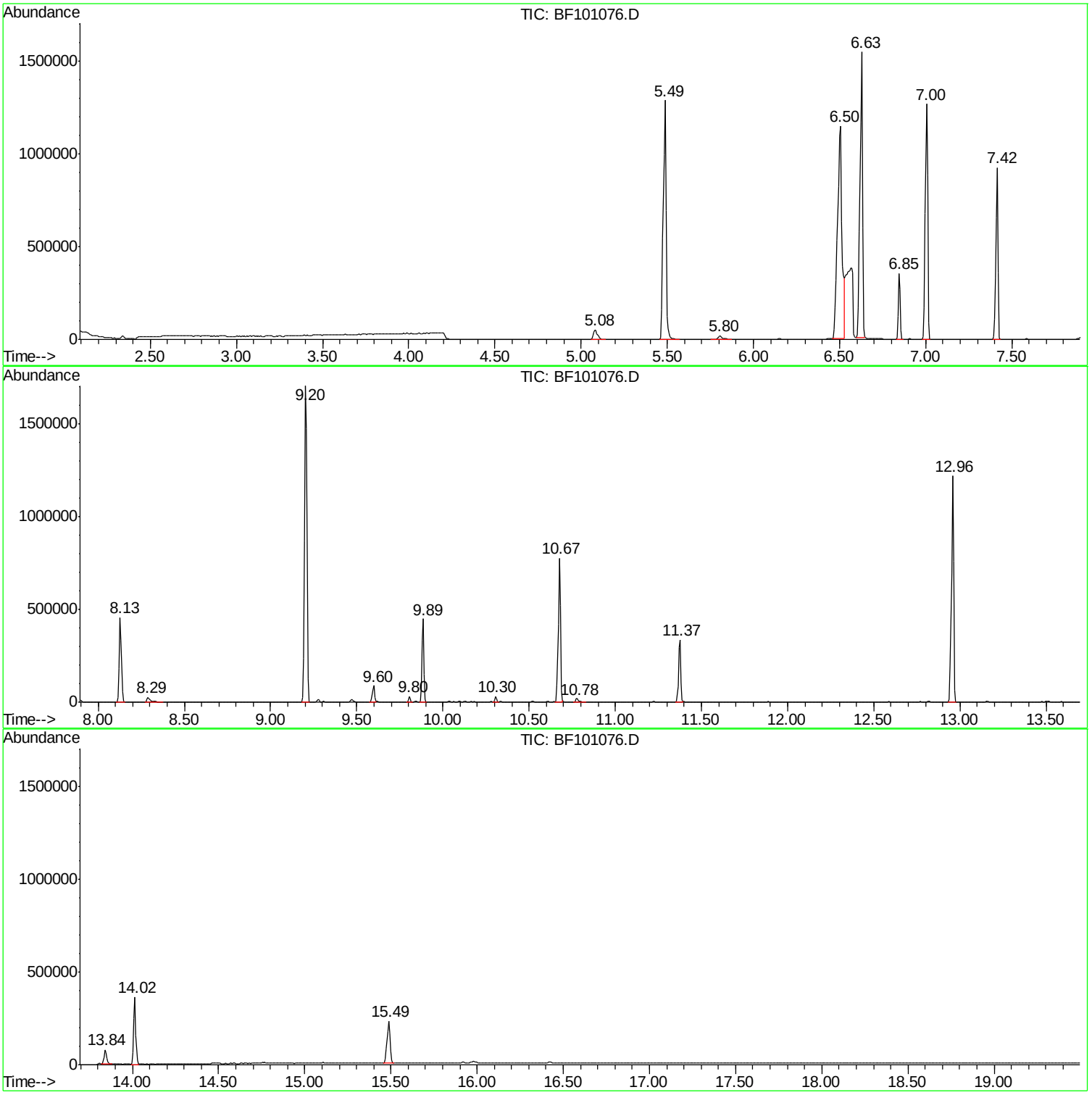
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBWW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF101076.D
Acq On : 1 Dec 2017 21:05
Operator : SJ/JU
Sample : I6622-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBWW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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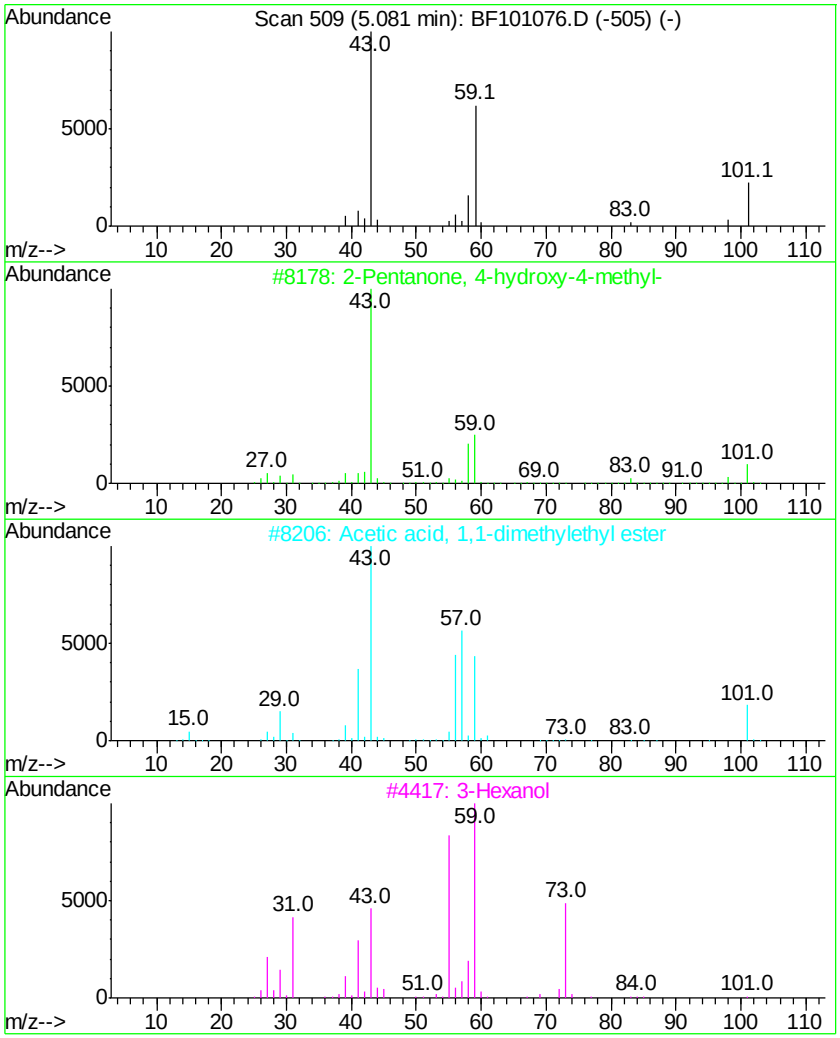
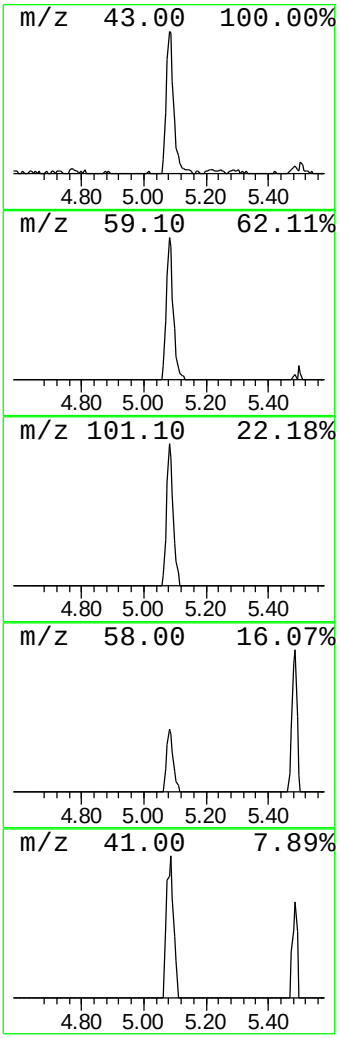
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	5.63 ng	81217	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Guanidine	59	CH5N3	000113-00-8	9
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9





Library Search Compound Report

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBWW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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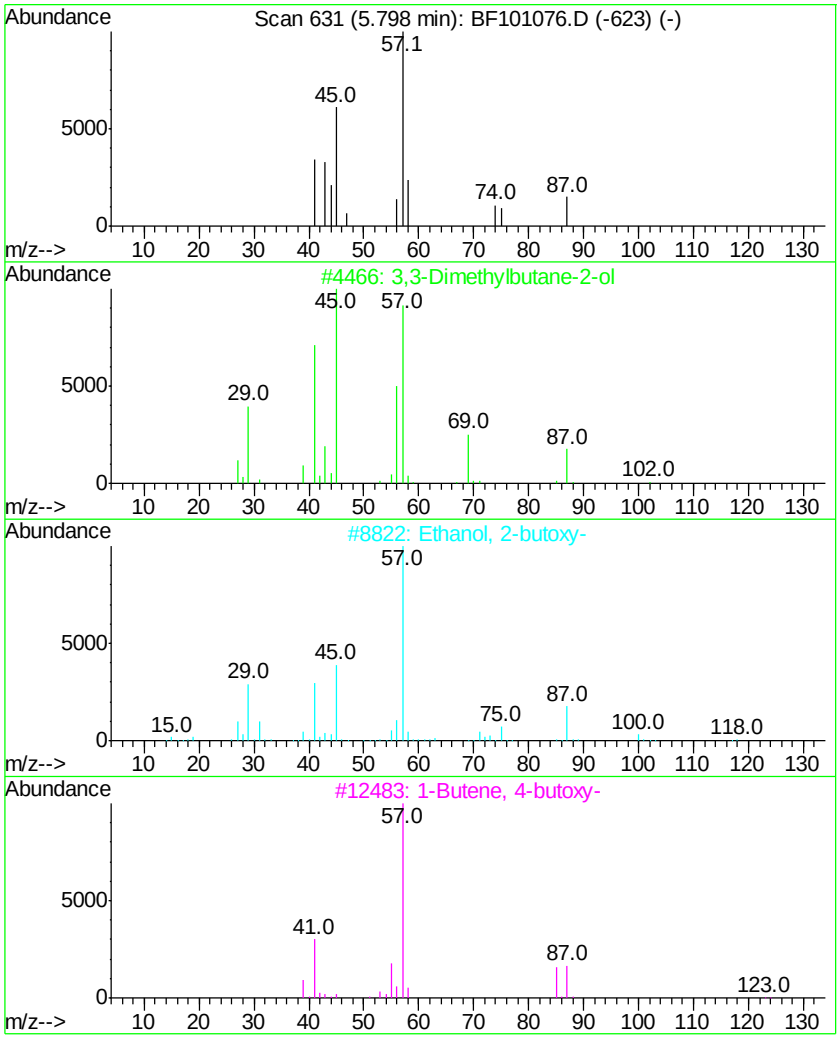
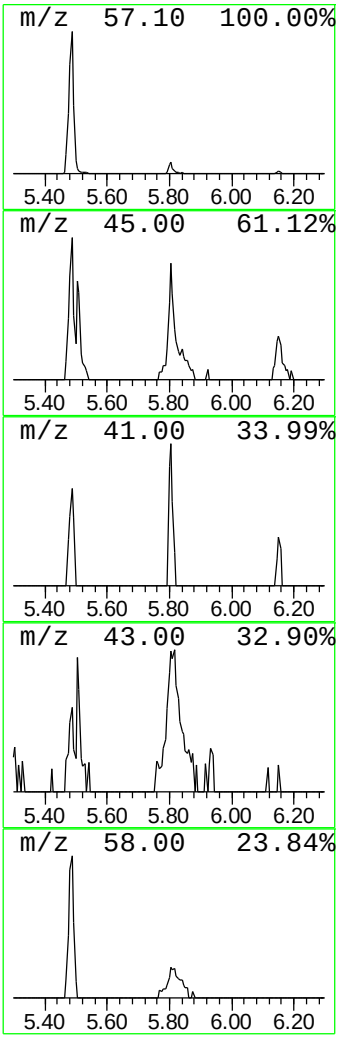
Peak Number 2 unknown5.80 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.80	2.49 ng	35848	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	36
2	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	9
3	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	9
4	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	9
5	Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	7





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Data File : BF101076.D
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Operator : SJ/JU
Sample : I6622-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBWW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Integration Parameters: LSCINT.P

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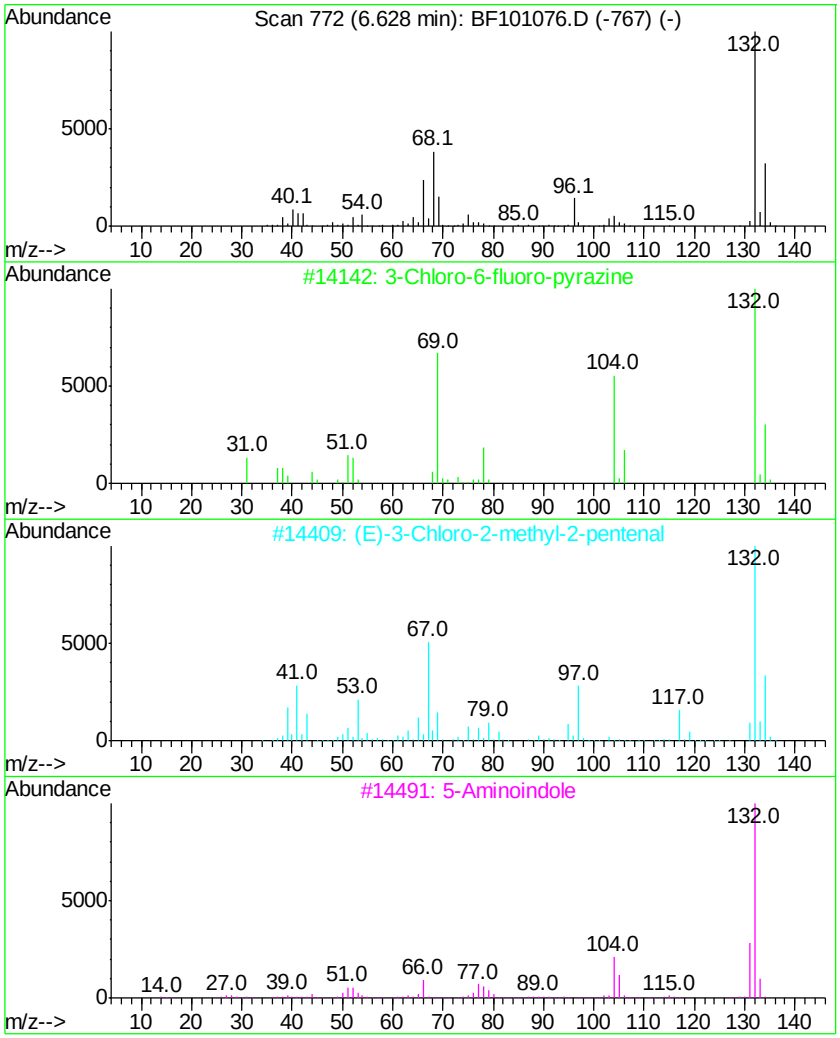
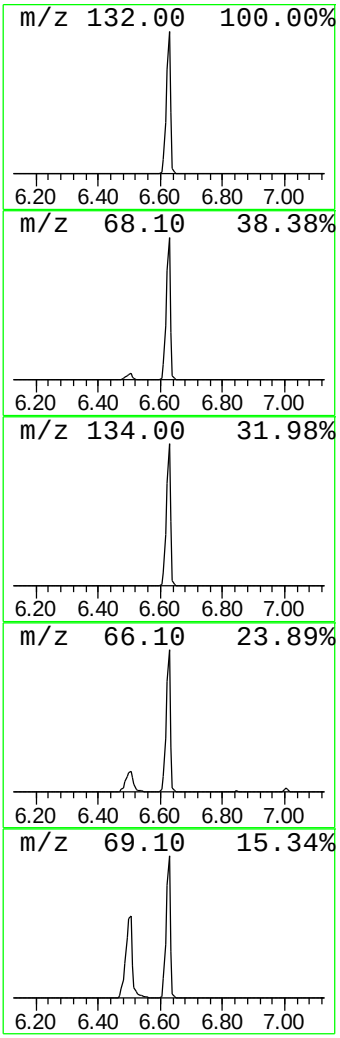
Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	100.00 ng	1441760	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument : BNA_F
ClientSampleId : DBWW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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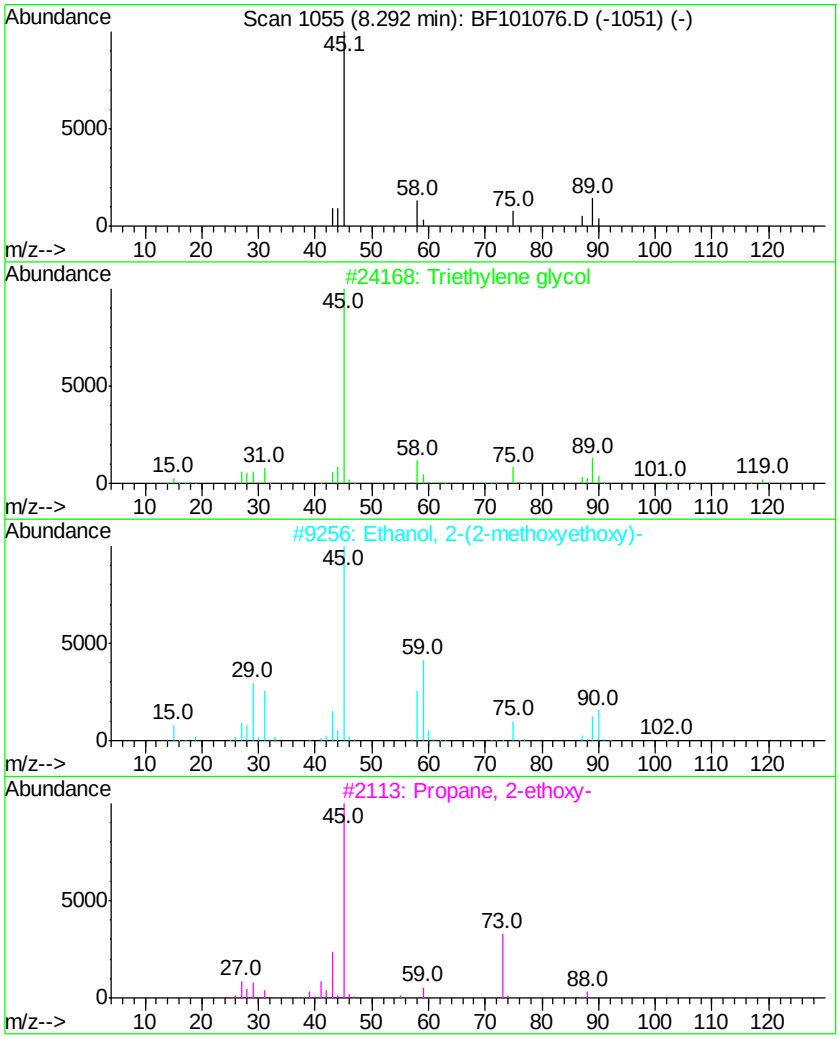
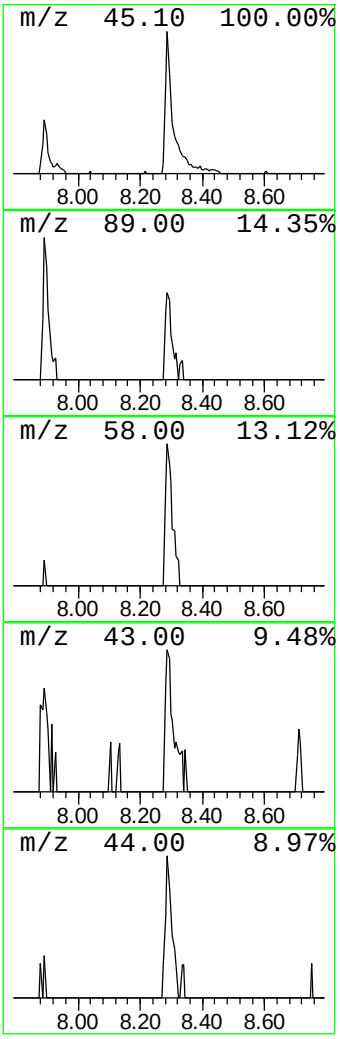
Peak Number 5 Triethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.29	2.31 ng	42778	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethylene glycol	150	C6H14O4	000112-27-6	83
2	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	39
3	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
4	Butane, 1-methoxy-	88	C5H12O	000628-28-4	9
5	Ethane, 1,2-dimethoxy-	90	C4H10O2	000110-71-4	9





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBWW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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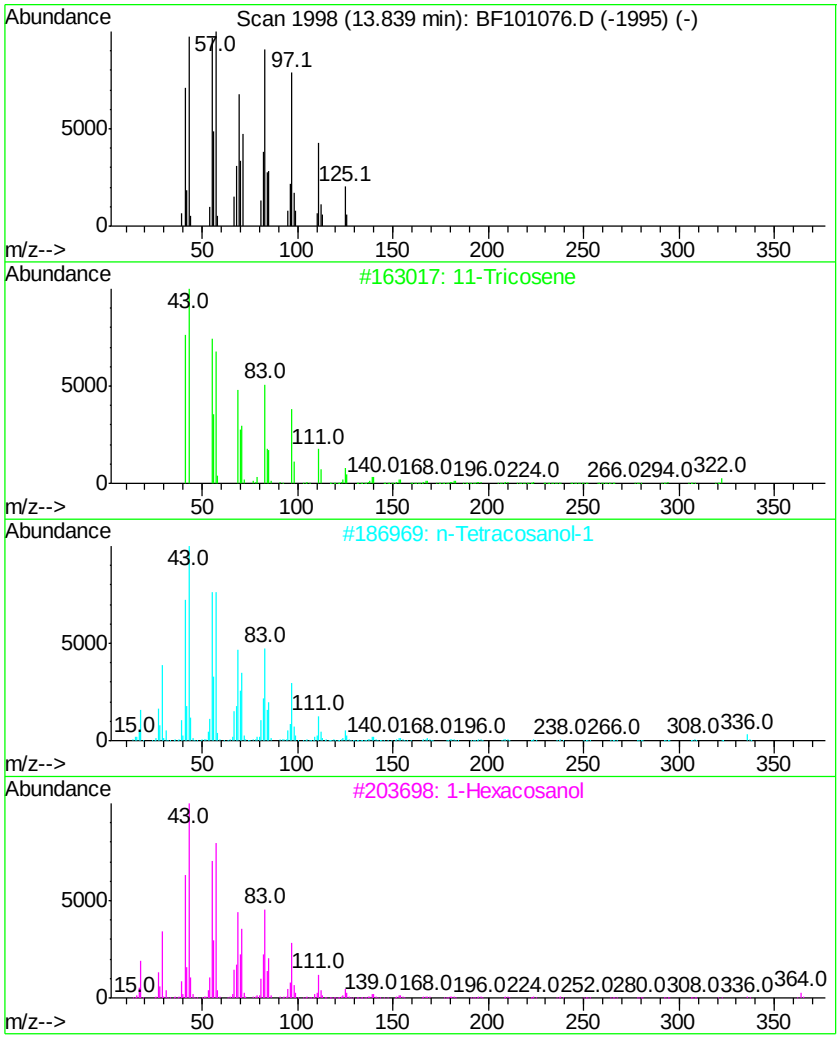
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

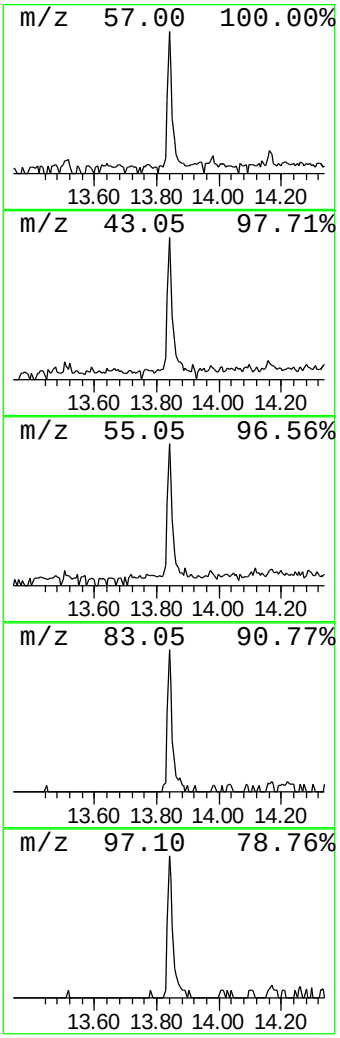
****

Peak Number 6 11-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	5.47 ng	83324	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	52
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	49
3	1-Hexacosanol	382	C26H54O	000506-52-5	46
4	Cyclotetradecane	196	C14H28	000295-17-0	43
5	1-Hexadecanol	242	C16H34O	036653-82-4	43





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	5.6	ng	81217	1	6.85	288363	20.0
unknown5.80	5.80	2.5	ng	35848	1	6.85	288363	20.0
unknown6.63	6.63	100.0	ng	1441760	1	6.85	288363	20.0
Triethylene glycol	8.29	2.3	ng	42778	2	8.13	370013	20.0
11-Tricosene	13.84	5.5	ng	83324	5	14.02	304689	20.0