LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104518.D
Acq On : 14 Apr 2018 11:06
Operator : JU/SJ
Sample : J2368-12
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-S

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-BF040618.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	5.004	492	496	502	rVB	151146	154936	3.56%	0.610%
2	5.422	563	567	579	rVB	1530141	1307024	30.02%	5.144%
3	6.028	667	670	681	rBV	95663	95852	2.20%	0.377%
4	6.439	736	740	747	rVB	858383	837865	19.25%	3.298%
5	6.575	759	763	767	rBV	2505974	2353974	54.07%	9.265%
6	6.633	769	773	776	rBV	536596	414655	9.52%	1.632%
7	6.810	799	803	806	rBV	963339	880012	20.21%	3.464%
8	6.969	825	830	833	rBV	3246110	3218186	73.92%	12.667%
9	7.375	893	899	902	rBV	2565674	2635567	60.54%	10.374%
10	8.092	1017	1021	1024	rBV	1392505	1137835	26.14%	4.478%
11	9.169	1198	1204	1207	rBV	4395009	4353644	100.00%	17.136%
12	9.557	1267	1270	1279	rBV	294738	272008	6.25%	1.071%
13	9.845	1314	1319	1329	rVB	1294106	1203961	27.65%	4.739%
14	10.274	1384	1392	1395	rBV2	60419	70102	1.61%	0.276%
15	10.639	1449	1454	1463	rVB	1513315	1501678	34.49%	5.911%
16	10.745	1470	1472	1482	rBV	55133	60333	1.39%	0.237%
17	11.333	1568	1572	1576	rBV	1038491	871628	20.02%	3.431%
18	12.739	1808	1811	1818	rBV2	102593	86437	1.99%	0.340%
19	12.927	1838	1843	1846	rBV	2812866	2655289	60.99%	10.451%
20	13.445	1928	1931	1934	rBV	62364	52803	1.21%	0.208%
21	13.815	1991	1994	2004	rBV	100671	127427	2.93%	0.502%
22	13.980	2018	2022	2025	rBV	648399	618205	14.20%	2.433%
23	15.439	2265	2270	2281	rBV	372405	497190	11.42%	1.957%

Sum of corrected areas: 25406611

LSC Report - Integrated Chromatogram

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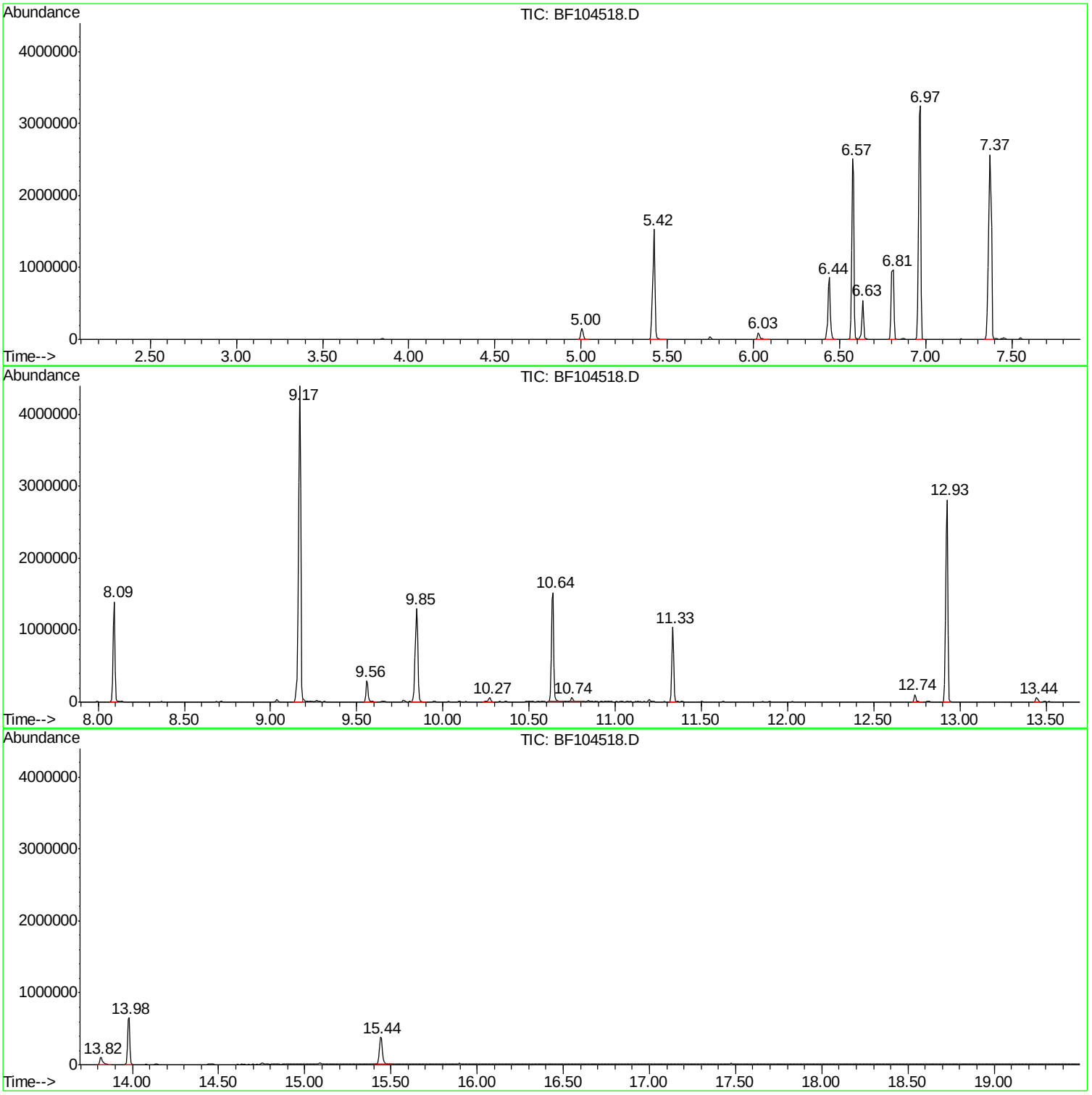
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104518.D
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Operator : JU/SJ
Sample : J2368-12
Misc :
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Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

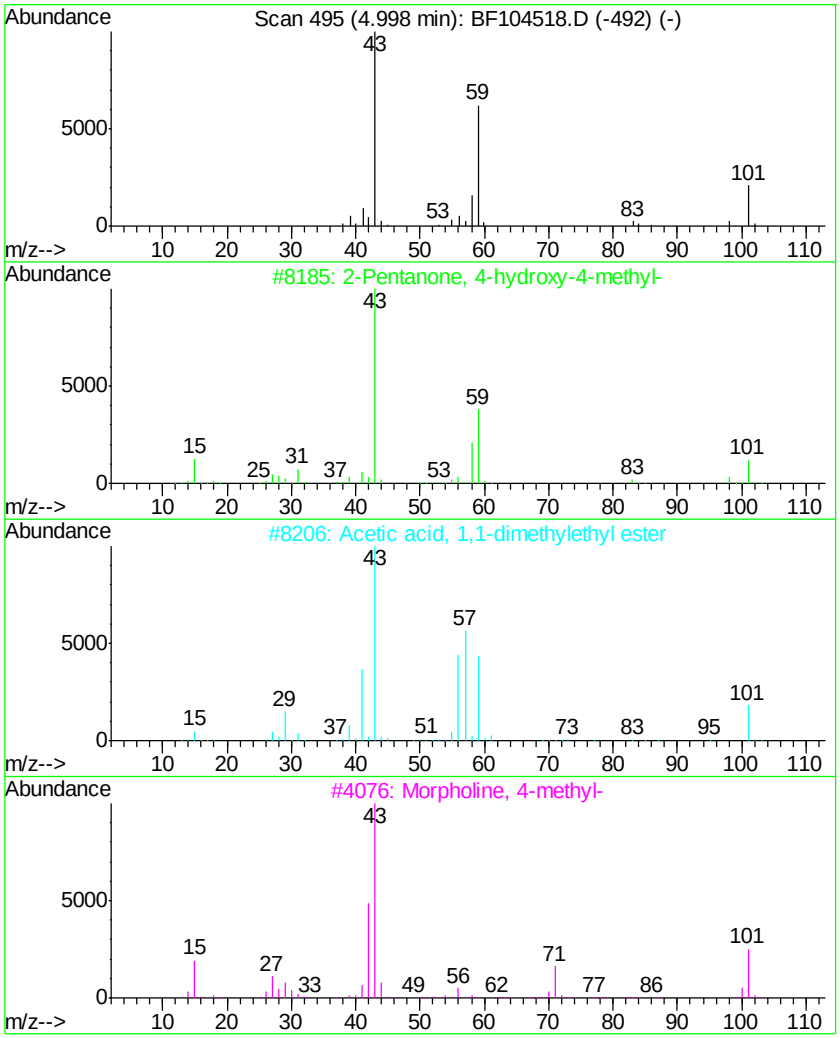
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

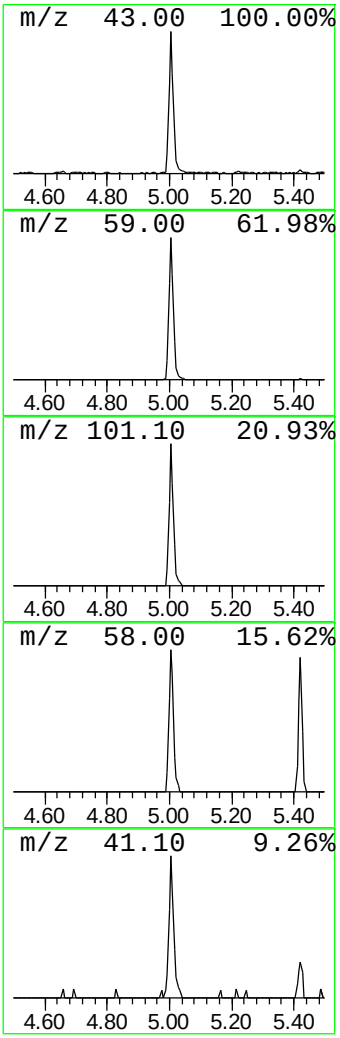
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.52 ng	154936	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9





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Sample : J2368-12
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

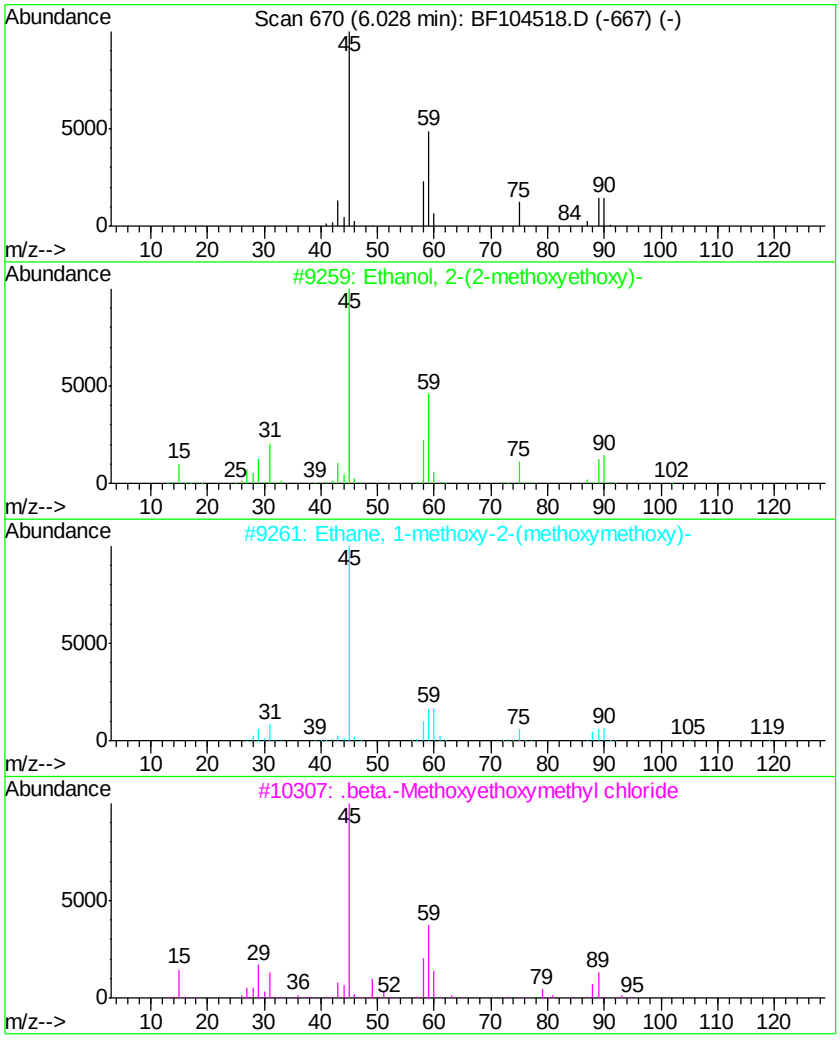
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

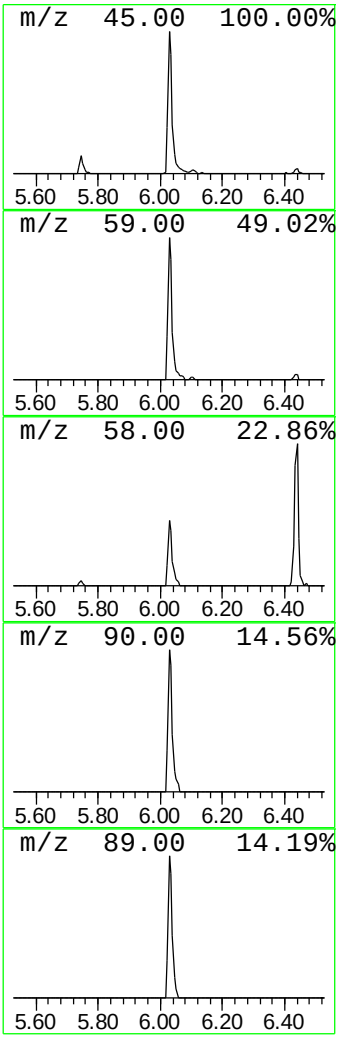
****

Peak Number 2 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.03	2.18 ng	95852	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	83
2	Ethane, 1-methoxy-2-(methoxymeth...	120	C5H12O3	074498-88-7	64
3	.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	50
4	Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	46
5	Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	38





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Data File : BF104518.D
Acq On : 14 Apr 2018 11:06
Operator : JU/SJ
Sample : J2368-12
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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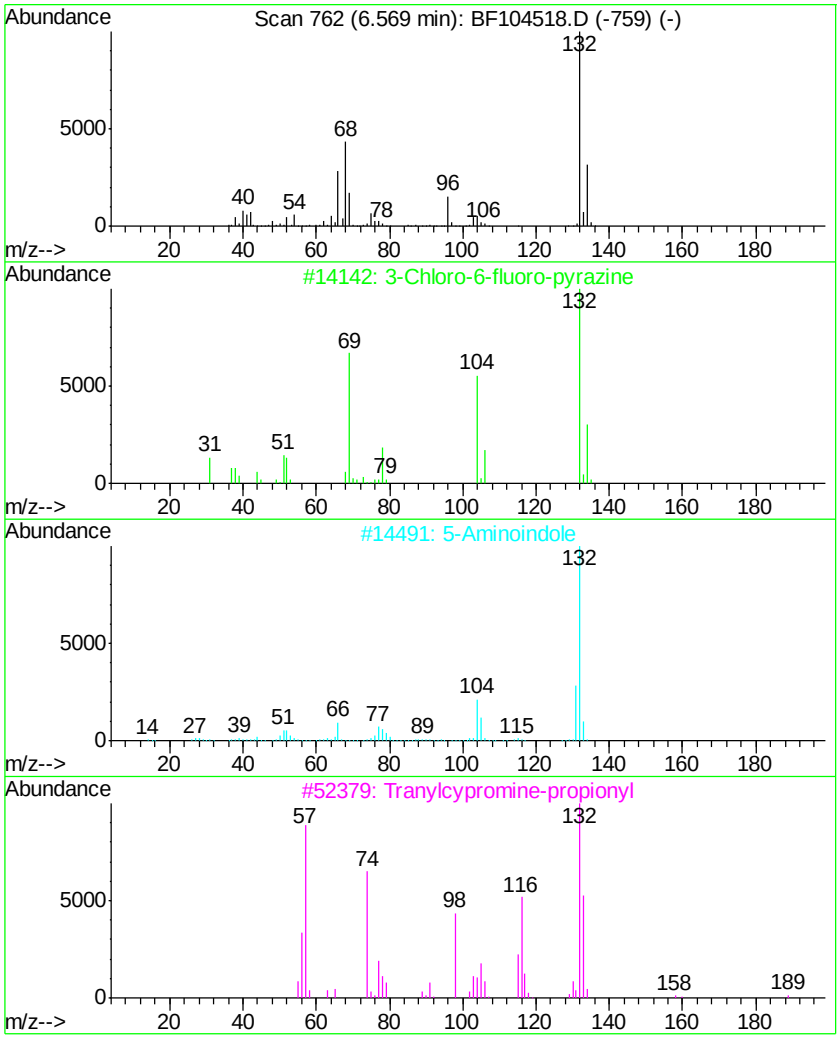
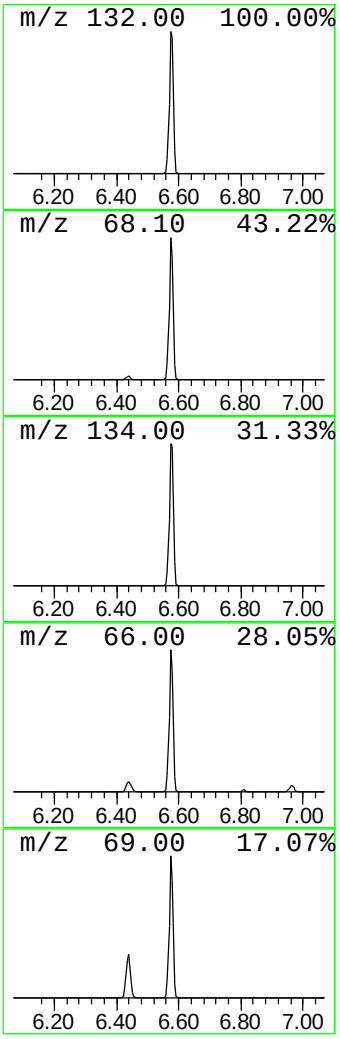
Peak Number 3 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	53.50 ng	2353970	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104518.D
Acq On : 14 Apr 2018 11:06
Operator : JU/SJ
Sample : J2368-12
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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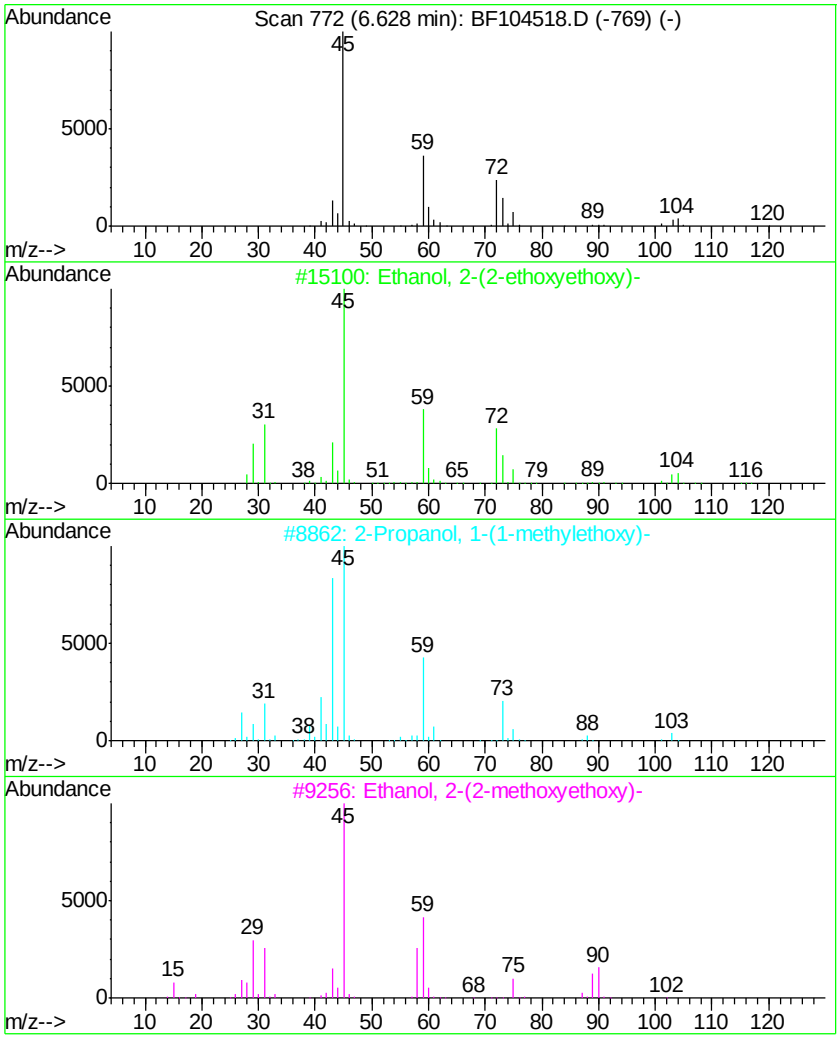
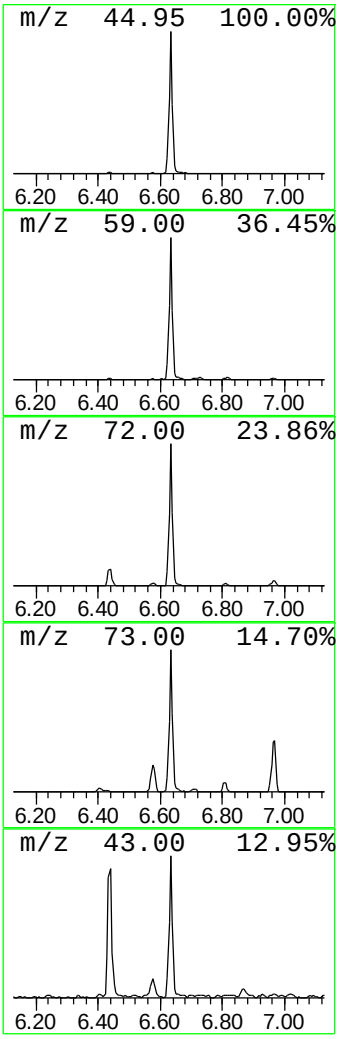
Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	9.42 ng	414655	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
3	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
4	Trimethylene glycol monomethyl e...	90	C4H10O2	001589-49-7	42
5	Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	38





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Sample : J2368-12
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

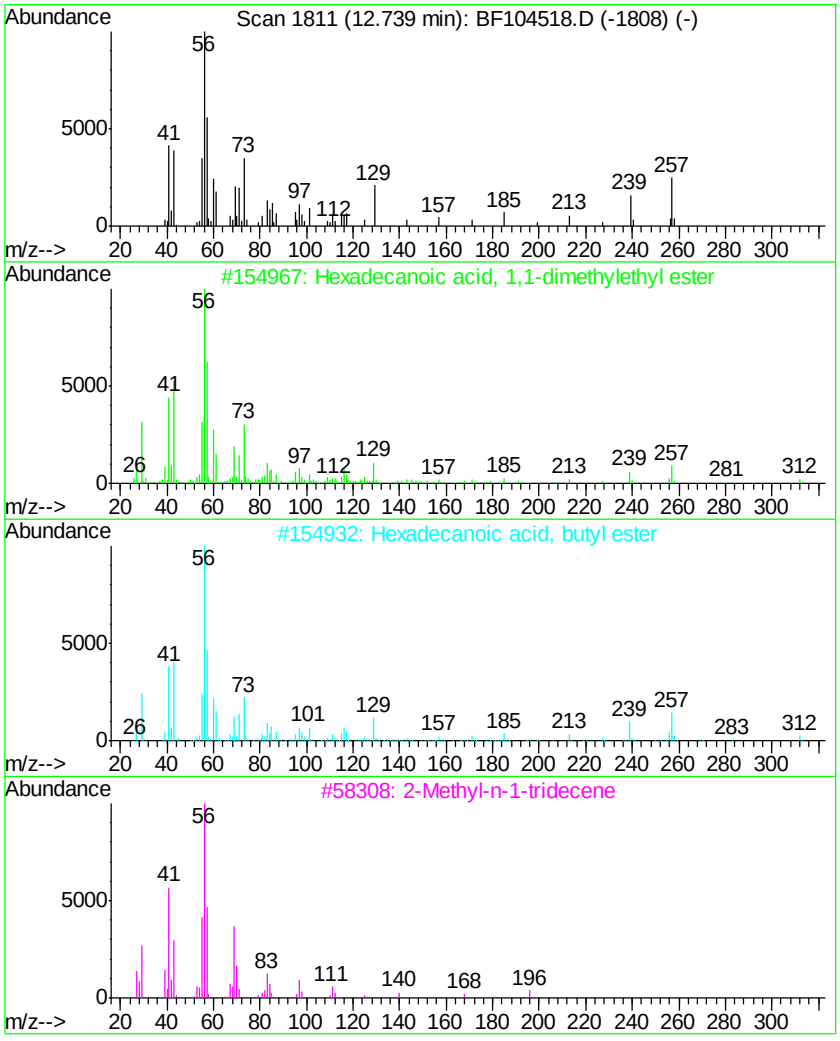
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

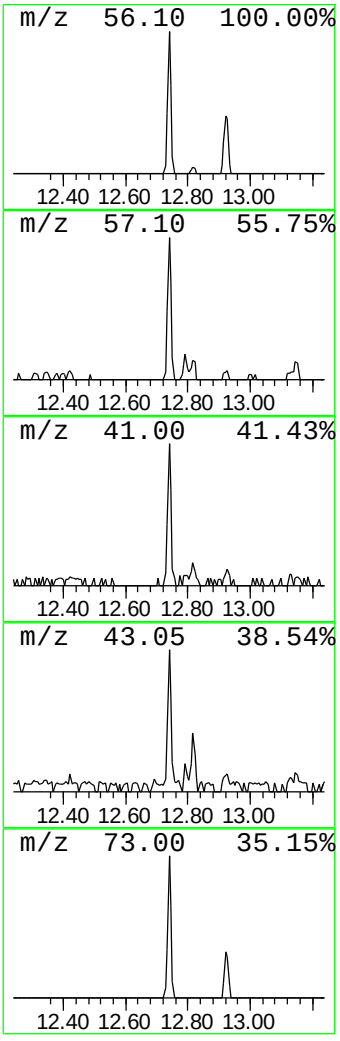
****

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.80 ng	86437	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	45
3	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	32
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30





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Sample : J2368-12
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRC-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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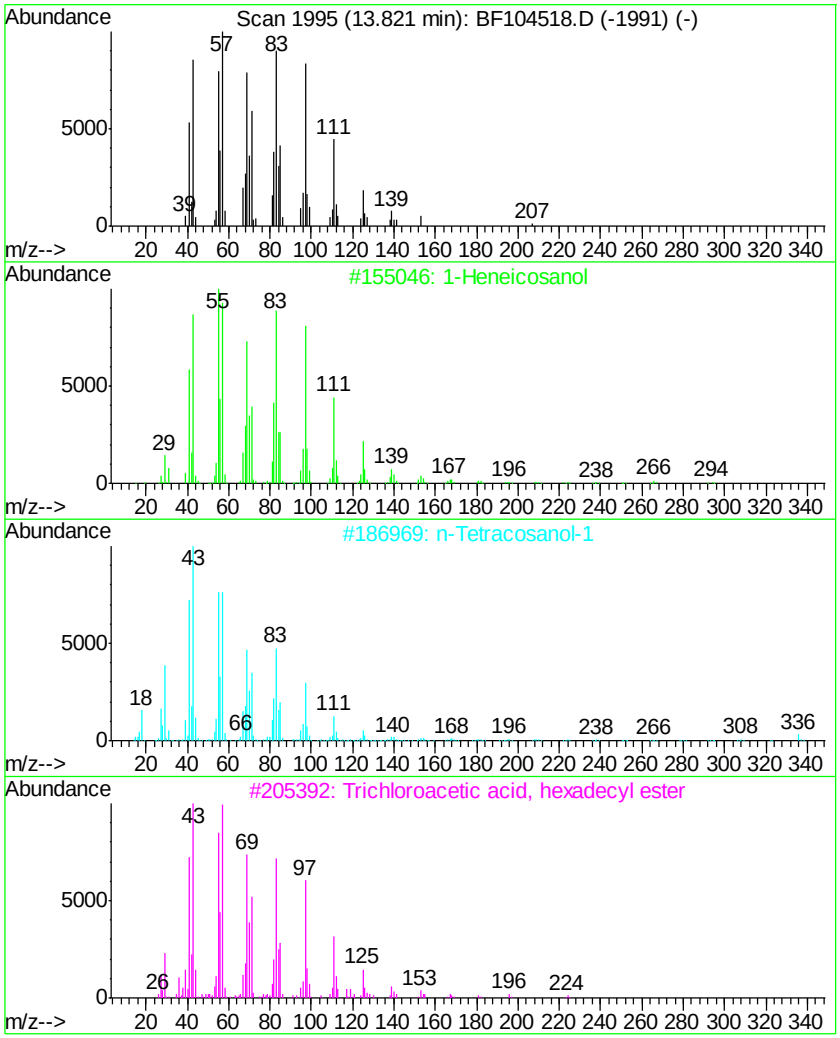
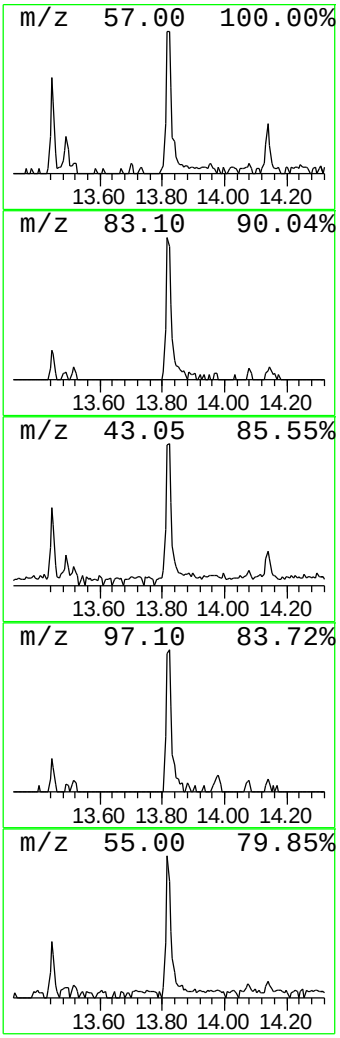
Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	4.12 ng	127427	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	3.5	ng	154936	1	6.81	880012	20.0
Ethanol, 2-(2-met...	6.03	2.2	ng	95852	1	6.81	880012	20.0
unknown6.57	6.57	53.5	ng	2353970	1	6.81	880012	20.0
Ethanol, 2-(2-eth...	6.63	9.4	ng	414655	1	6.81	880012	20.0
Hexadecanoic acid...	12.74	2.8	ng	86437	5	13.98	618205	20.0
1-Heneicosanol	13.82	4.1	ng	127427	5	13.98	618205	20.0