LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081516\
Data File : BG023726.D
Acq On : 15 Aug 2016 18:28
Operator : UM/SJ
Sample : H4422-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

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_G\Methods\8270-BG080116.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	5.654	472	479	490	rBV	1427288	2729668	3.37%	0.902%
2	7.281	749	756	781	rBV	746271	2047613	2.53%	0.676%
3	7.639	809	817	831	rBV3	2701044	6748435	8.33%	2.229%
4	7.886	850	859	869	rBV	6506220	12224245	15.09%	4.037%
5	8.092	885	894	905	rBV	3586662	6592380	8.14%	2.177%
6	8.438	942	953	962	rBV	2089591	3697598	4.57%	1.221%
7	9.290	1090	1098	1108	rVB	1944279	3619146	4.47%	1.195%
8	10.941	1371	1379	1392	rBV	876953	1625571	2.01%	0.537%
9	11.986	1548	1557	1568	rBV	878198	2424486	2.99%	0.801%
10	12.121	1570	1580	1584	rVV	4473093	10560372	13.04%	3.488%
11	12.192	1584	1592	1596	rVV	6604913	21402717	26.43%	7.069%
12	12.239	1596	1600	1614	rVV	8540614	18748557	23.15%	6.192%
13	12.427	1614	1632	1635	rVV	19658017	80989283	100.00%	26.749%
14	12.480	1636	1641	1643	rVV2	23593096	46088458	56.91%	15.222%
15	12.503	1643	1645	1659	rVV	5922501	7119188	8.79%	2.351%
16	12.680	1659	1675	1679	rVV	16859379	43703732	53.96%	14.435%
17	13.402	1789	1798	1807	rBV	5026627	8250924	10.19%	2.725%
18	14.788	2027	2034	2041	rBV2	1340380	2206595	2.72%	0.729%
19	16.286	2282	2289	2302	rVB	3498494	5585486	6.90%	1.845%
20	17.549	2498	2504	2514	rVB2	1393945	2128432	2.63%	0.703%
21	18.419	2647	2652	2659	rBV2	551813	973495	1.20%	0.322%
22	19.694	2864	2869	2885	rBV	1254757	2259543	2.79%	0.746%
23	20.158	2943	2948	2956	rVB	5034198	6953435	8.59%	2.297%
24	21.873	3234	3240	3248	rVB2	1225371	2149168	2.65%	0.710%
25	25.280	3811	3820	3831	rVB3	665814	1942300	2.40%	0.642%

Sum of corrected areas: 302770827

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Misc :
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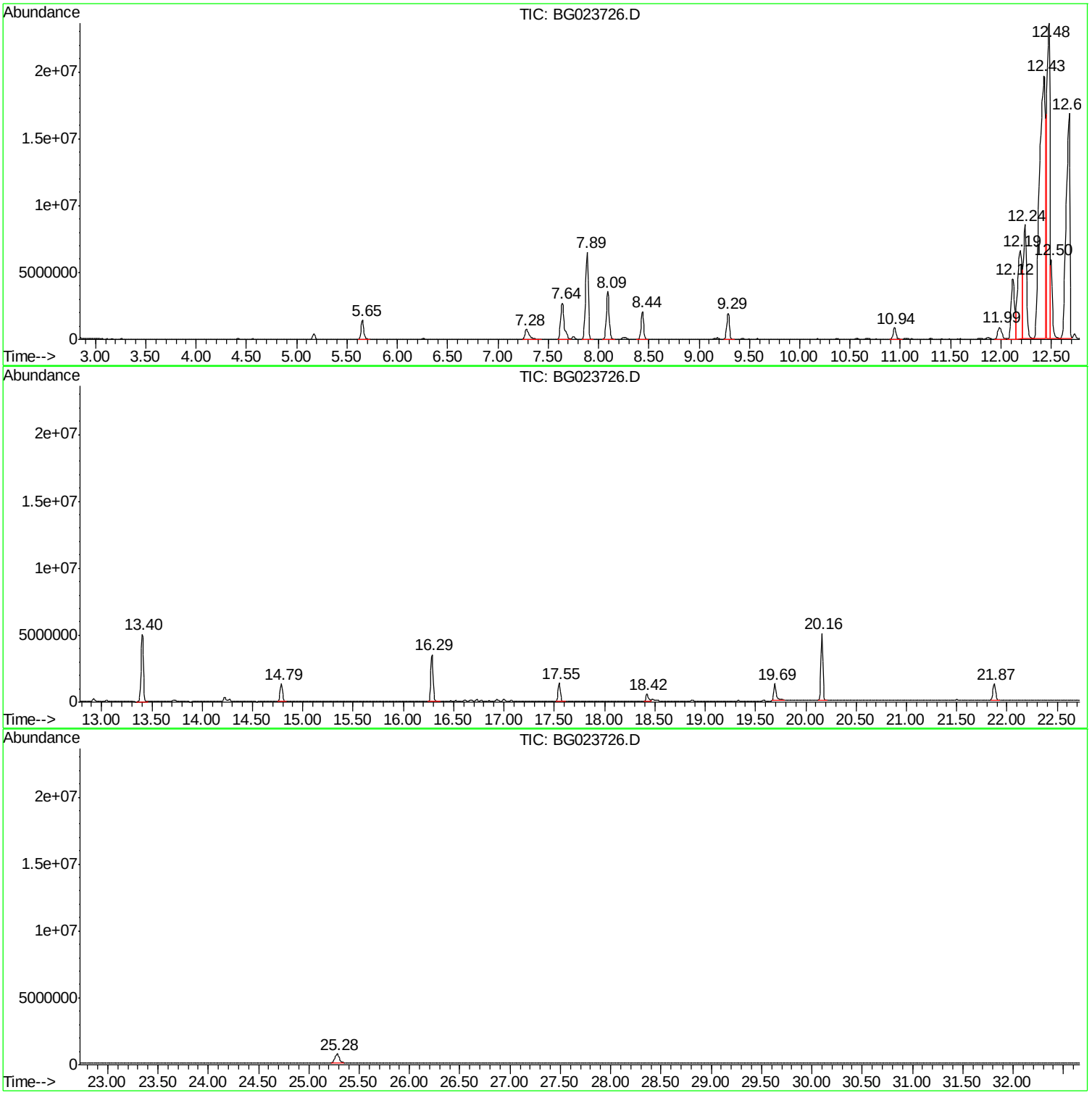
Instrument :
BNA_G
ClientSampleId :
MW-1

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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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Operator : UM/SJ
Sample : H4422-03
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Instrument : BNA_G
ClientSampleId : MW-1

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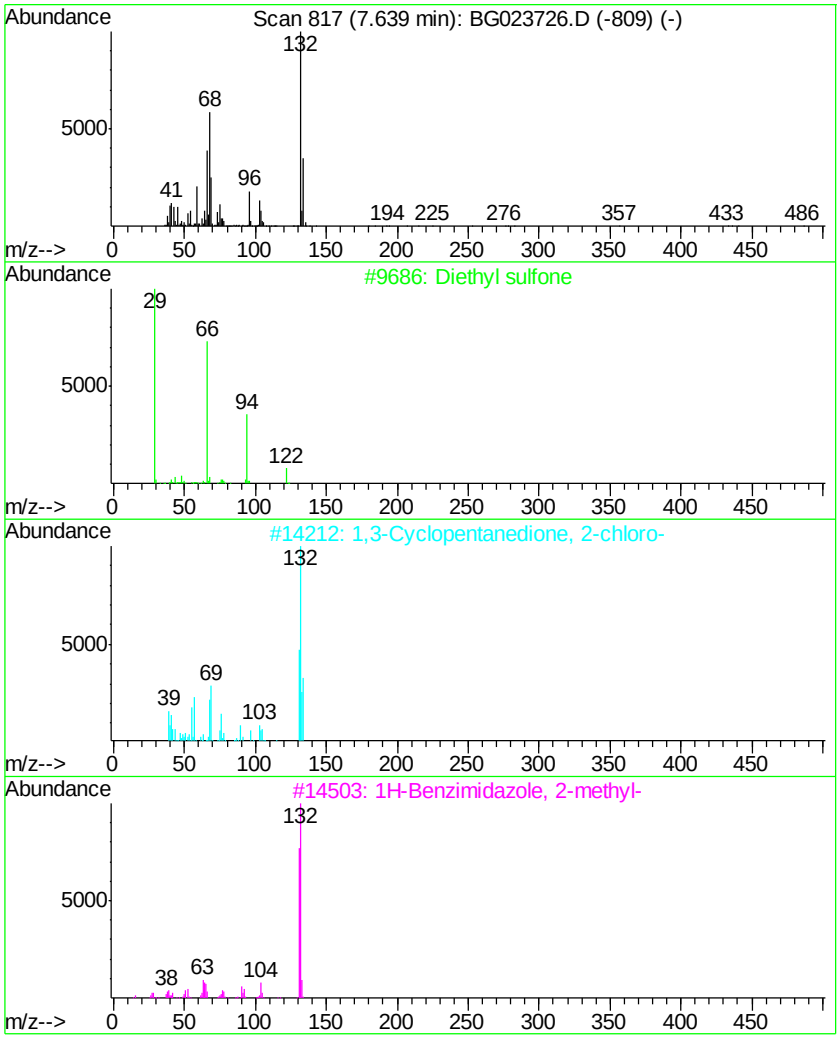
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

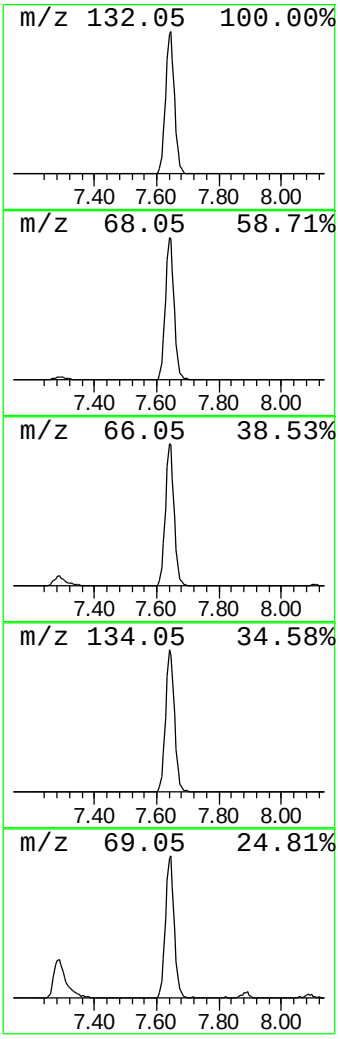
****

Peak Number 1 unknown7.64 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	20.47 ng	6748440	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl sulfone	122	C4H10O2S	000597-35-3	17
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	11
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
5	3H-1,2-Dithiol-3-one, 4-methyl-	132	C4H4OS2	003620-10-8	10





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Operator : UM/SJ
Sample : H4422-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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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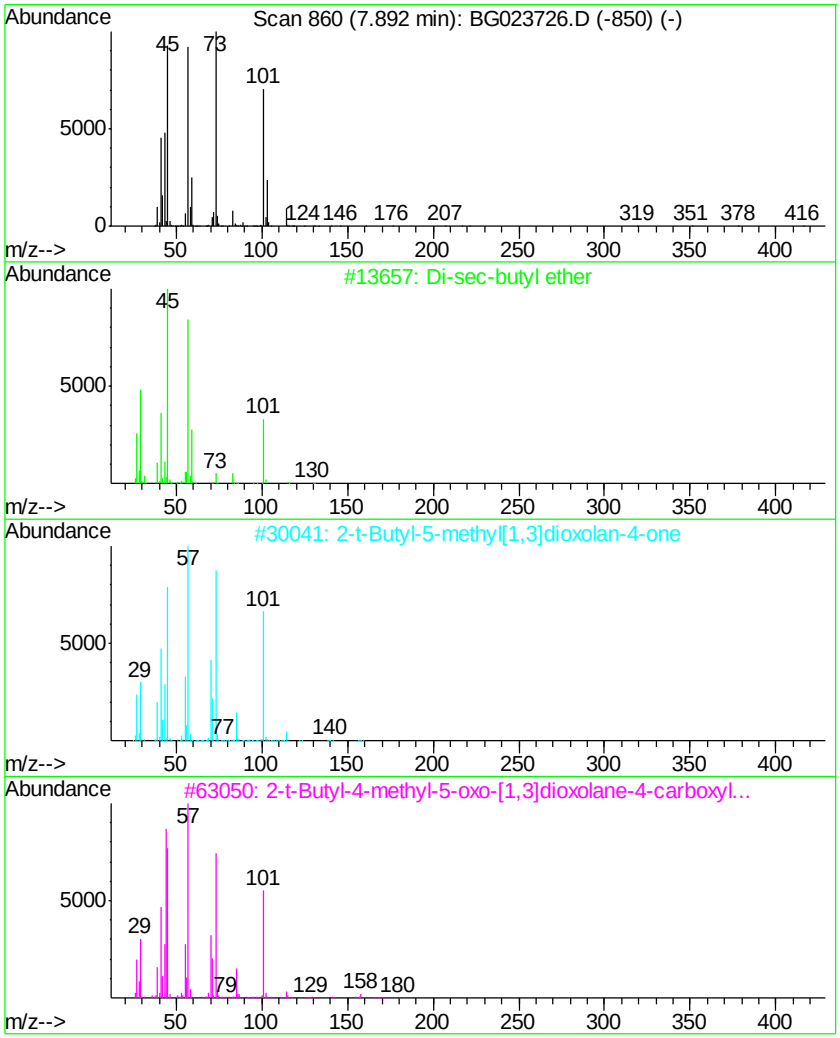
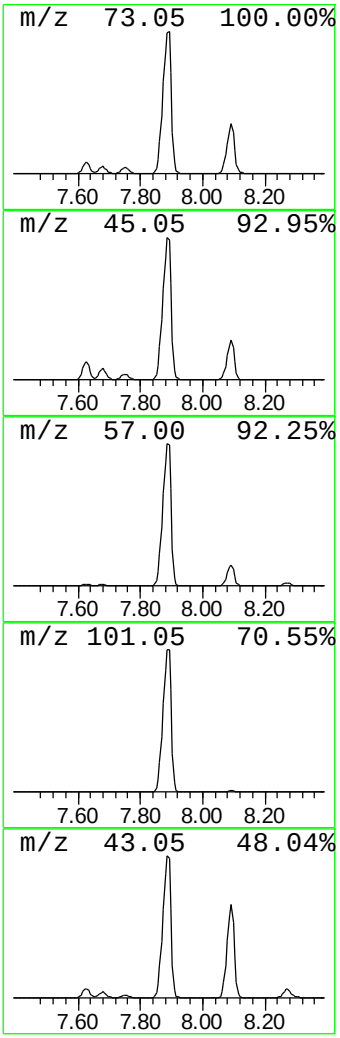
Peak Number 2 Di-sec-butyl ether Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.89	37.09 ng	12224200	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-butyl ether	130	C8H18O	006863-58-7	59
2	2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	45
3	2-t-Butyl-4-methyl-5-oxo-[1,3]di...	202	C9H14O5	1000191-45-5	45
4	2-Methylbutane-1,4-diol, 3-(1-et...	192	C9H20O4	088481-54-3	37
5	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	33





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Data File : BG023726.D
Acq On : 15 Aug 2016 18:28
Operator : UM/SJ
Sample : H4422-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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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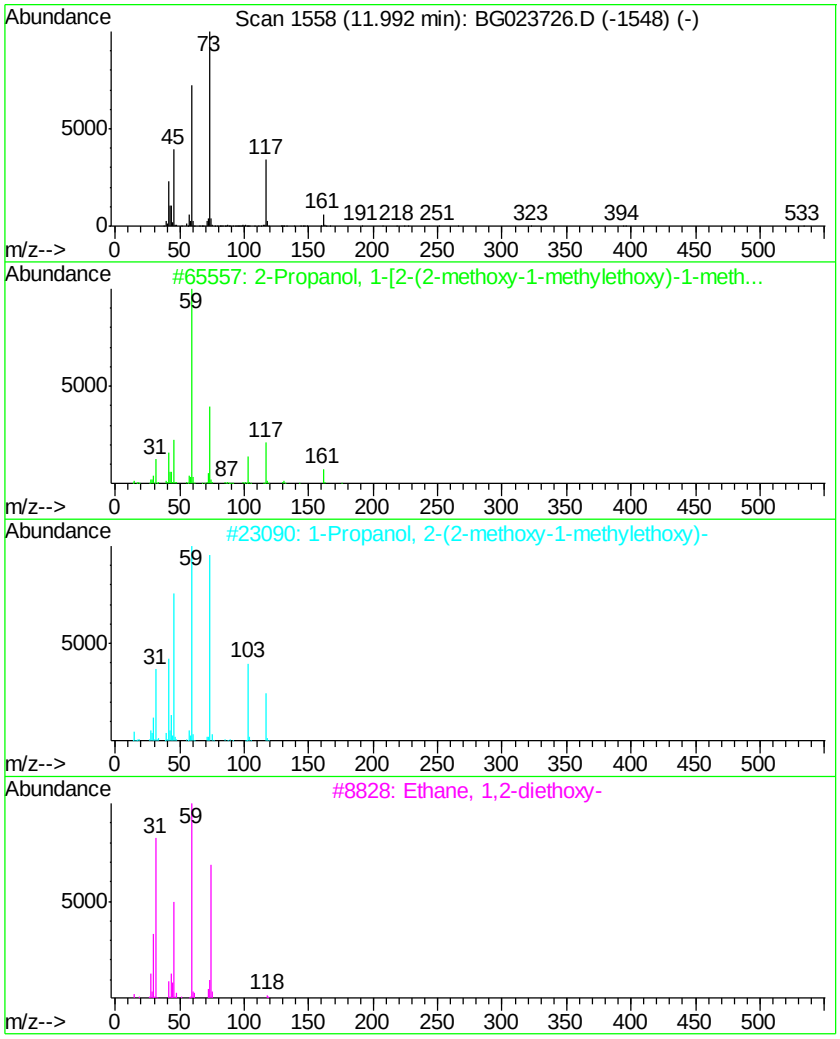
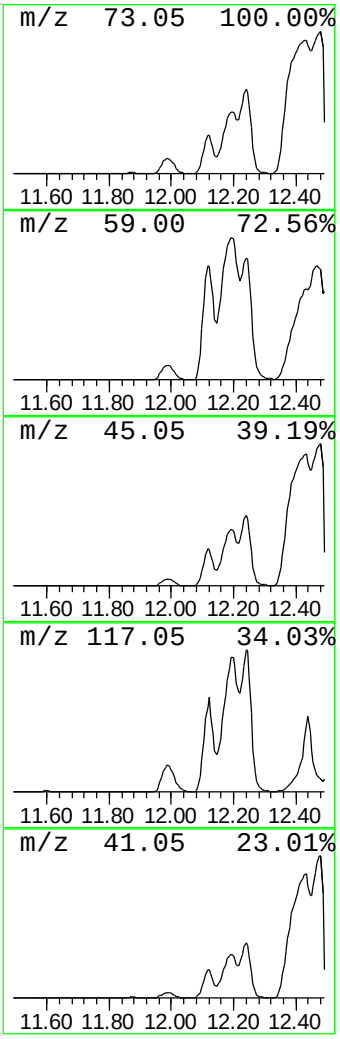
Peak Number 4 2-Propanol, 1-[2-(2-methoxy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	29.83 ng	2424490	Naphthalene-d8	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	50
2	1-Propanol, 2-(2-methoxy-1-methy...	148	C7H16O3	055956-21-3	50
3	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	47
4	1,3-Dioxolane, 2-ethyl-	102	C5H10O2	002568-96-9	38
5	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	38





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081516\
Data File : BG023726.D
Acq On : 15 Aug 2016 18:28
Operator : UM/SJ
Sample : H4422-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.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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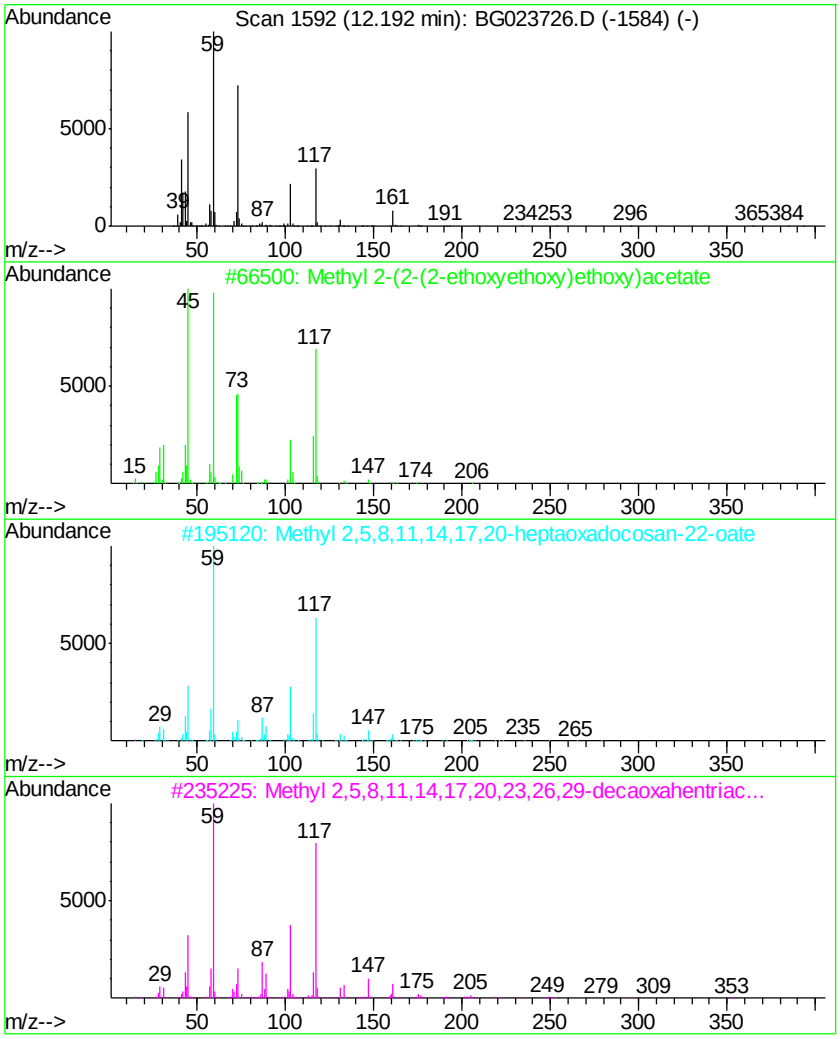
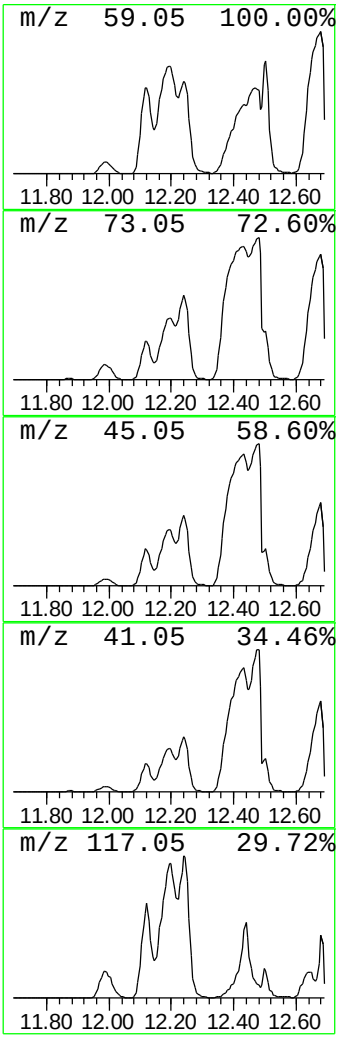
Peak Number 6 Methyl 2-(2-(2-ethoxyethoxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.19	263.33 ng	21402700	Naphthalene-d8	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 2-(2-(2-ethoxyethoxy)etho...	206	C9H18O5	1000366-78-1	72
2	Methyl 2,5,8,11,14,17,20-heptaox...	368	C16H32O9	1000366-81-3	64
3	Methyl 2,5,8,11,14,17,20,23,26,2...	500	C22H44O12	1000366-81-0	64
4	Tri(1,2-propyleneglycol), monome...	206	C10H22O4	1000262-26-6	56
5	Silane, dimethyl-	60	C2H8Si	001111-74-6	53





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081516\
Data File : BG023726.D
Acq On : 15 Aug 2016 18:28
Operator : UM/SJ
Sample : H4422-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

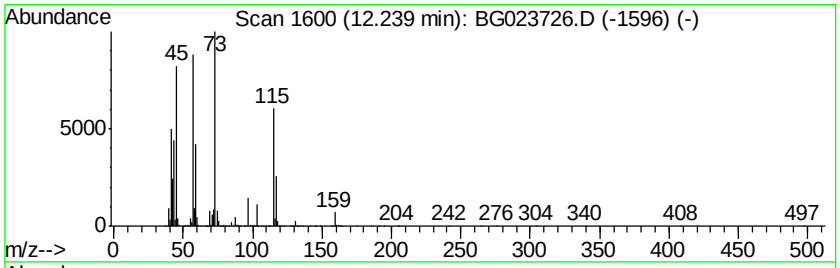
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

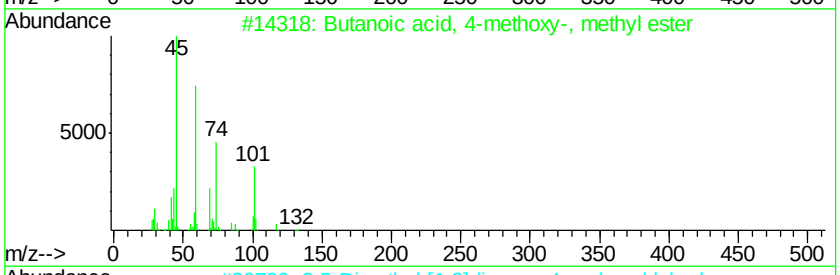
****

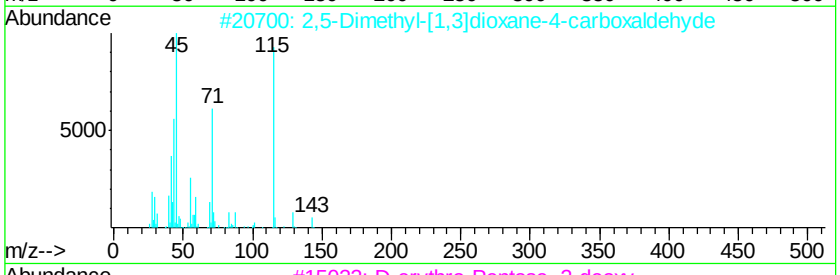
Peak Number 7 unknown12.24 Concentration Rank 5

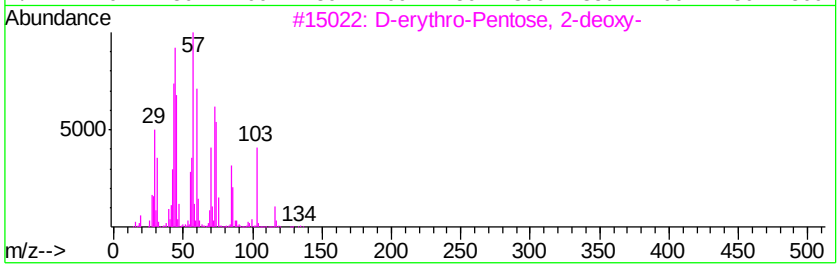
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.24	230.67 ng	18748600	Naphthalene-d8	10.94

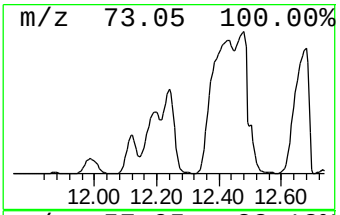
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	35
2	2,5-Dimethyl-[1,3]dioxane-4-carb...	144	C7H12O3	1000188-14-4	32
3	D-erythro-Pentose, 2-deoxy-	134	C5H10O4	000533-67-5	27
4	Acetic acid, (2-ethoxy)ethoxy-, ...	162	C7H14O4	016326-34-4	25
5	1H-Pyrimidine-2,4-dione, 1-(2-et...	232	C9H13FN2O4	1000310-13-7	25

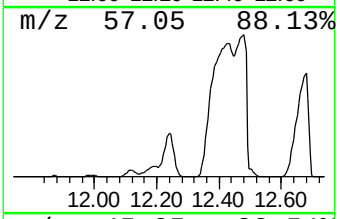


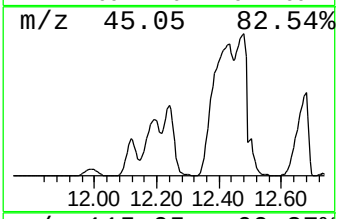


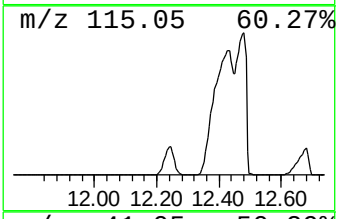


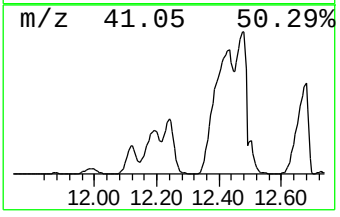












Library Search Compound Report

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Sample : H4422-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

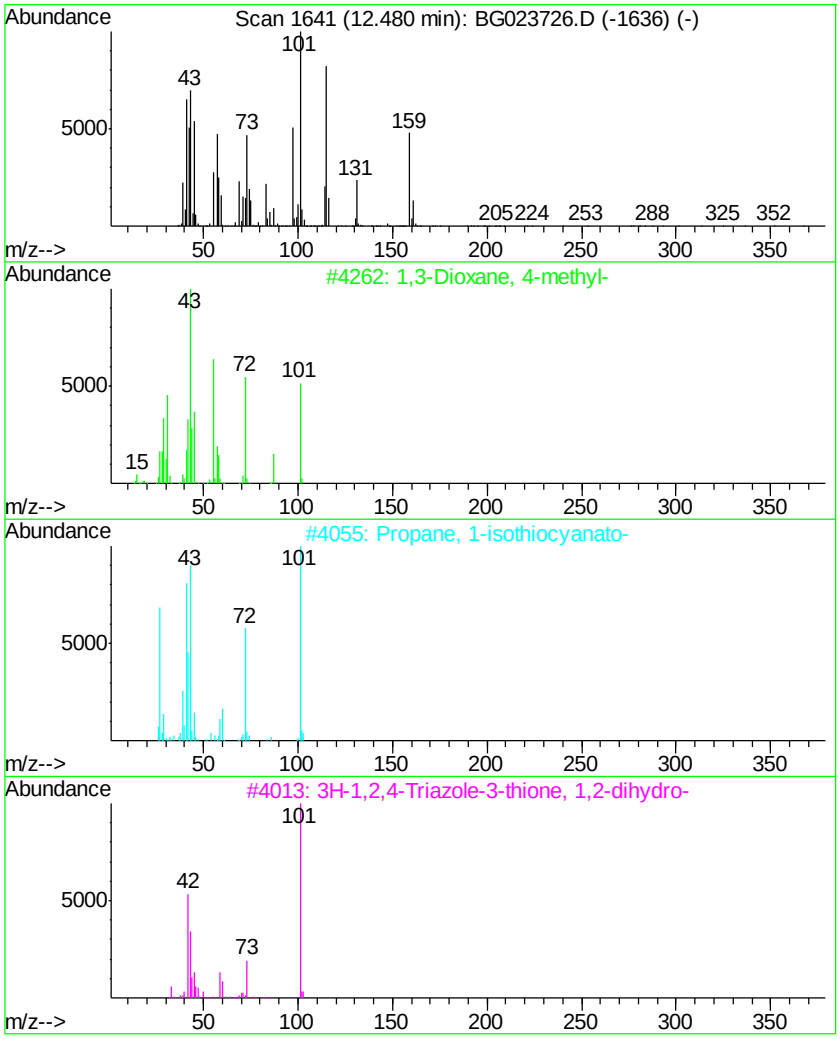
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

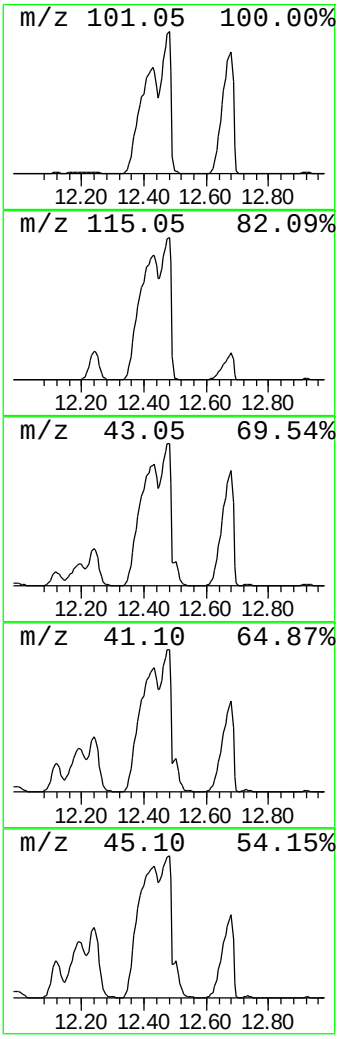
****

Peak Number 9 unknown12.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	567.04 ng	46088500	Naphthalene-d8	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	27
2	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	25
3	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	22
4	1,3,4-Thiadiazol-2-amine	101	C2H3N3S	004005-51-0	22
5	Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	22





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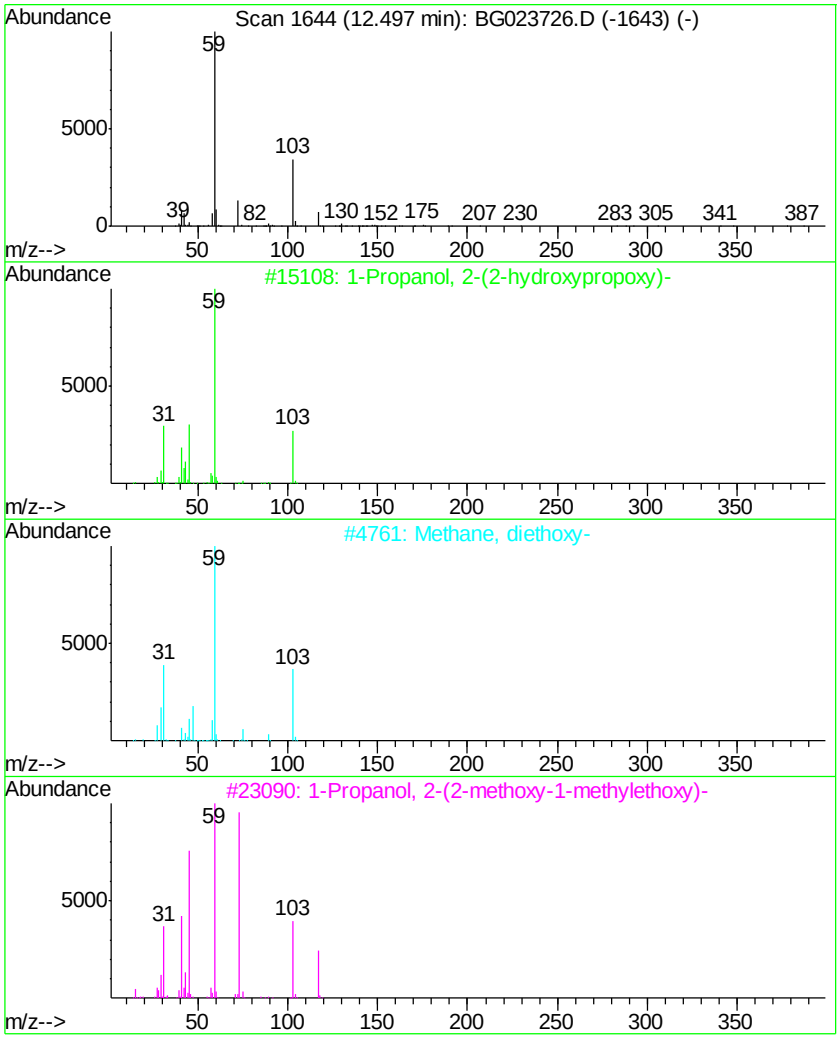
TIC Integration Parameters: LSCINT.P

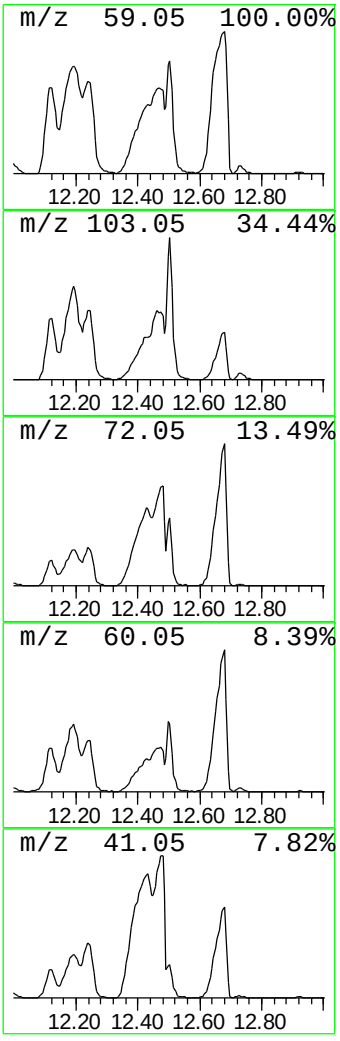
****

Peak Number 10 1-Propanol, 2-(2-hydroxypro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	87.59 ng	7119190	Naphthalene-d8	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
2	Methane, diethoxy-	104	C5H12O2	000462-95-3	50
3	1-Propanol, 2-(2-methoxy-1-methy...	148	C7H16O3	055956-21-3	40
4	1-(1-Methoxypropan-2-yloxy)propa...	230	C12H22O4	1000367-11-3	33
5	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-13-4	33





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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

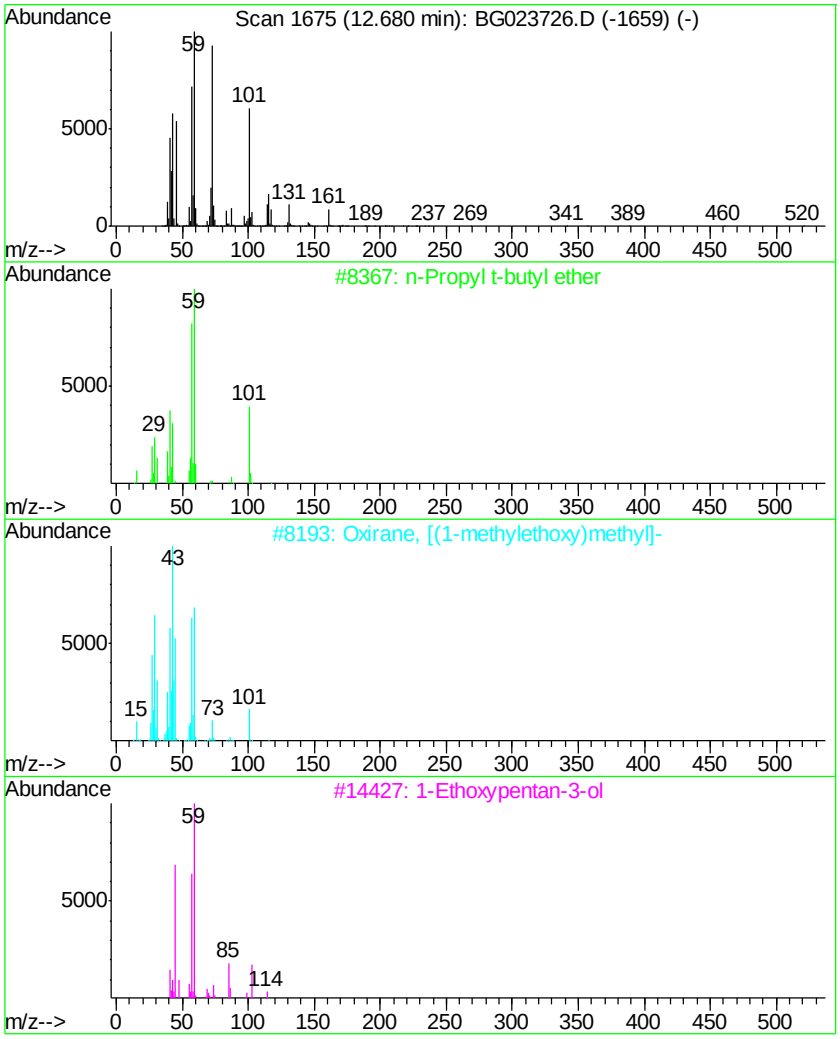
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

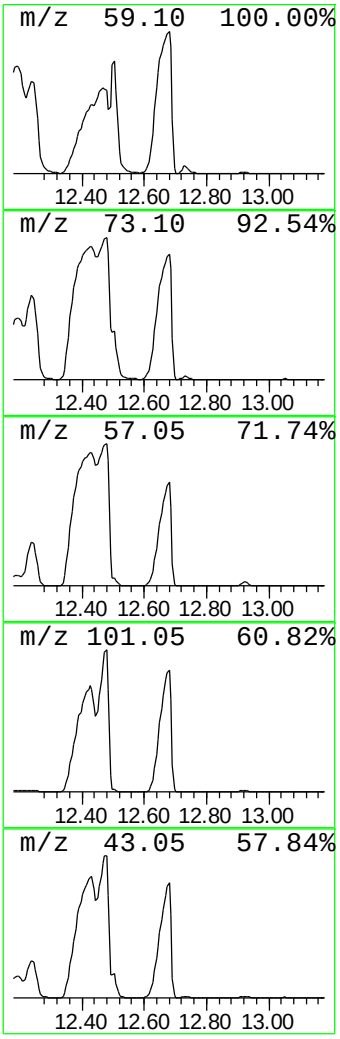
****

Peak Number 11 unknown12.68 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	537.70 ng	43703700	Naphthalene-d8	10.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	43
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	38
3	1-Ethoxypentan-3-ol	132	C7H16O2	100910-92-7	35
4	Butanal, oxime	87	C4H9NO	000110-69-0	27
5	3-Hexanol, 3-ethyl-	130	C8H18O	000597-76-2	25





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081516\
Data File : BG023726.D
Acq On : 15 Aug 2016 18:28
Operator : UM/SJ
Sample : H4422-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

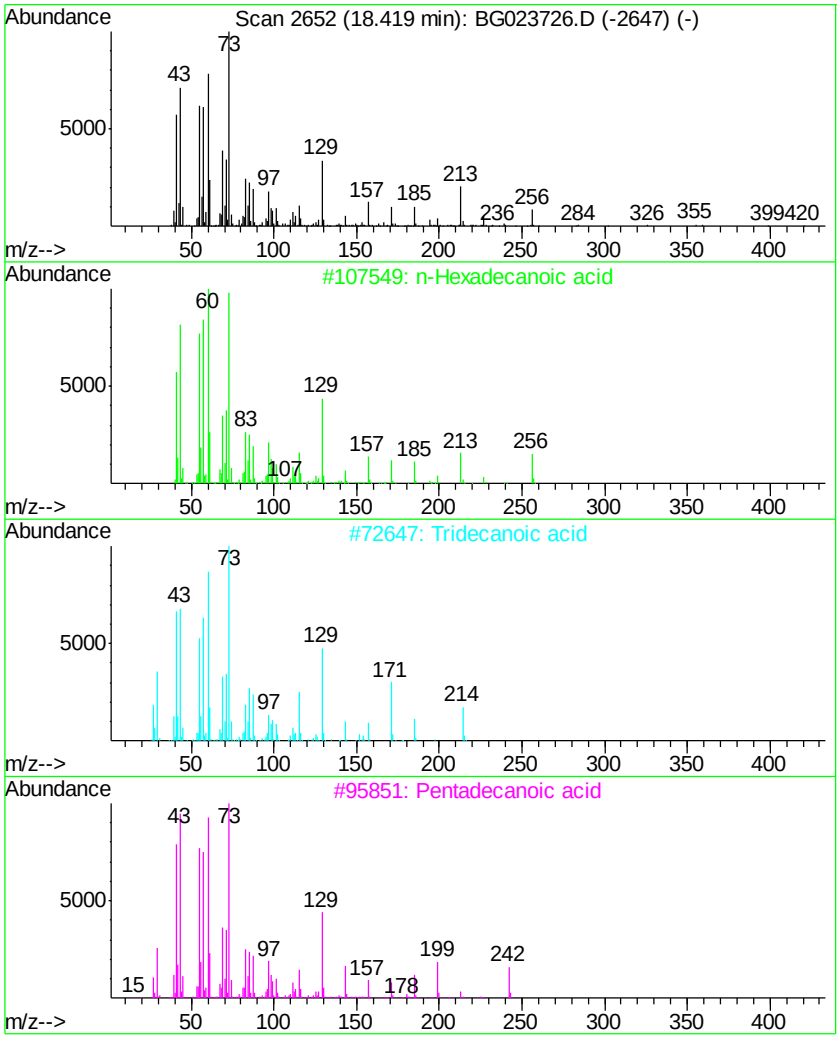
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

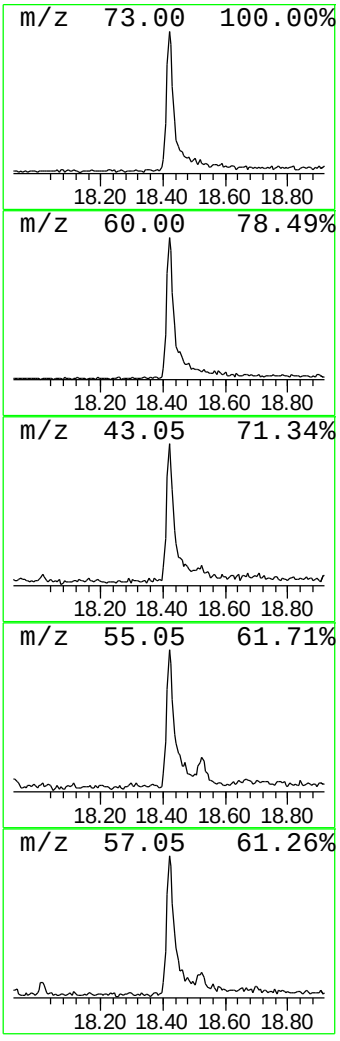
****

Peak Number 12 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	9.15 ng	973495	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	58





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081516\
Data File : BG023726.D
Acq On : 15 Aug 2016 18:28
Operator : UM/SJ
Sample : H4422-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

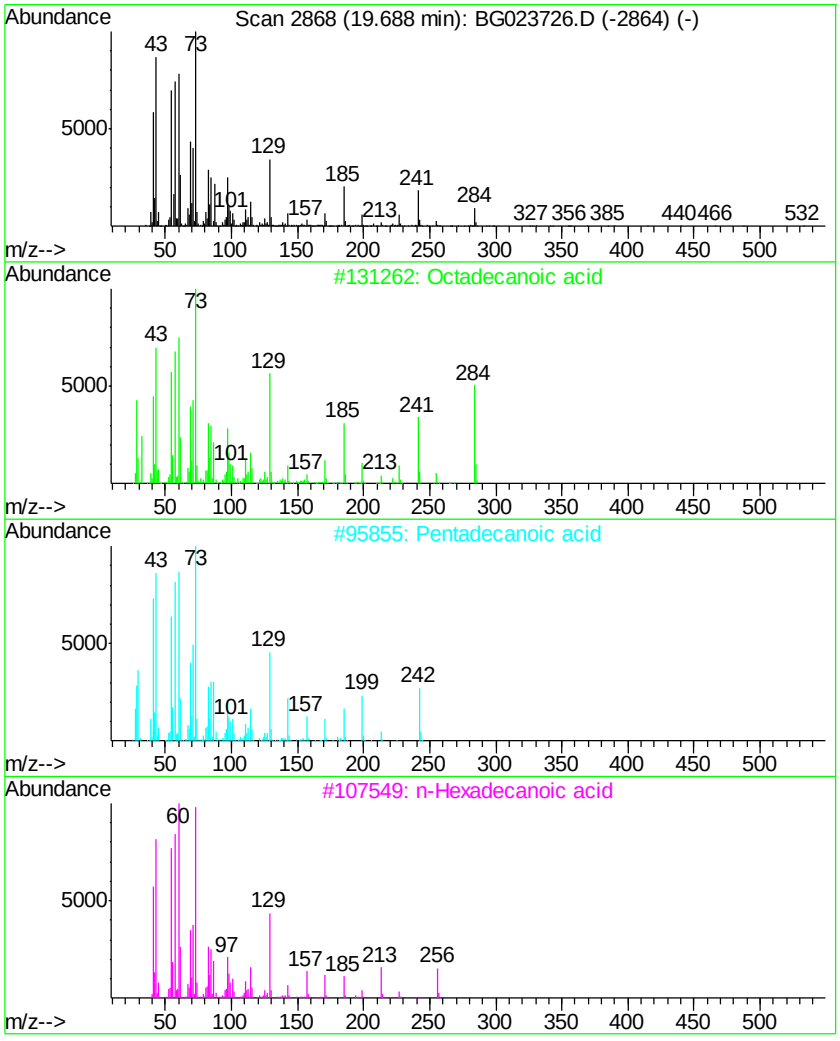
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

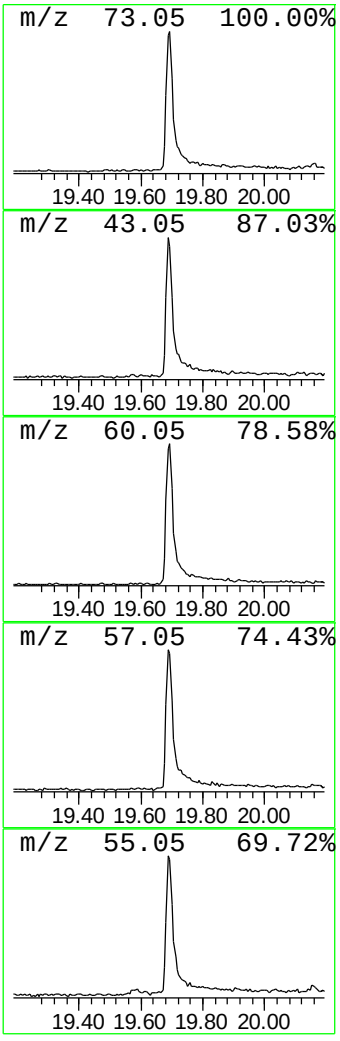
****

Peak Number 13 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	21.23 ng	2259540	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG081516\
Data File : BG023726.D
Acq On : 15 Aug 2016 18:28
Operator : UM/SJ
Sample : H4422-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-1

Quant Method : Z:\HPCHEM1\BNA_G\Methods\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.64	7.64	20.5	ng	6748440	1	8.11	6592380	20.0
Di-sec-butyl ether	7.89	37.1	ng	12224200	1	8.11	6592380	20.0
2-Propanol, 1-[2-...	11.99	29.8	ng	2424490	2	10.94	1625570	20.0
Methyl 2-(2-(2-et...	12.19	263.3	ng	21402700	2	10.94	1625570	20.0
unknown12.24	12.24	230.7	ng	18748600	2	10.94	1625570	20.0
unknown12.48	12.48	567.0	ng	46088500	2	10.94	1625570	20.0
1-Propanol, 2-(2-...	12.50	87.6	ng	7119190	2	10.94	1625570	20.0
unknown12.68	12.68	537.7	ng	43703700	2	10.94	1625570	20.0
n-Hexadecanoic acid	18.42	9.2	ng	973495	4	17.55	2128430	20.0
Octadecanoic acid	19.69	21.2	ng	2259540	4	17.55	2128430	20.0