LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037502.D
Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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	5.544	376	384	395	rBV	1218715	1993520	3.90%	2.017%
2	5.750	410	419	429	rVB	337449	791650	1.55%	0.801%
3	6.267	480	507	511	rBV2	9201600	51142950	100.00%	51.756%
4	7.254	663	675	685	rBV2	360722	761781	1.49%	0.771%
5	7.636	730	740	749	rBV	889412	1615013	3.16%	1.634%
6	8.429	868	875	894	rVB	716576	1359208	2.66%	1.375%
7	9.281	970	1020	1030	rBV2	2541728	17706294	34.62%	17.918%
8	10.926	1293	1300	1308	rVB	342725	652189	1.28%	0.660%
9	12.189	1507	1515	1523	rBV2	279934	811302	1.59%	0.821%
10	13.359	1708	1714	1723	rBV	1647410	2697243	5.27%	2.730%
11	13.676	1762	1768	1772	rBV	987550	1556601	3.04%	1.575%
12	14.739	1943	1949	1957	rVB2	536484	887361	1.74%	0.898%
13	15.151	2013	2019	2026	rBV2	498935	900984	1.76%	0.912%
14	16.238	2195	2204	2210	rBV2	2000038	4000983	7.82%	4.049%
15	17.483	2411	2416	2422	rBV2	631231	1024846	2.00%	1.037%
16	18.300	2550	2555	2560	rBV	1488804	2034344	3.98%	2.059%
17	18.347	2560	2563	2576	rVB3	430598	625063	1.22%	0.633%
18	19.957	2833	2837	2848	rVB	1087233	1389693	2.72%	1.406%
19	20.086	2853	2859	2865	rVB	2448811	3299875	6.45%	3.339%
20	21.349	3069	3074	3089	rVB2	493305	1120128	2.19%	1.134%
21	21.772	3140	3146	3154	rVB	627395	1104537	2.16%	1.118%
22	25.104	3702	3713	3730	rVB3	387837	1340723	2.62%	1.357%

Sum of corrected areas: 98816288

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037502.D
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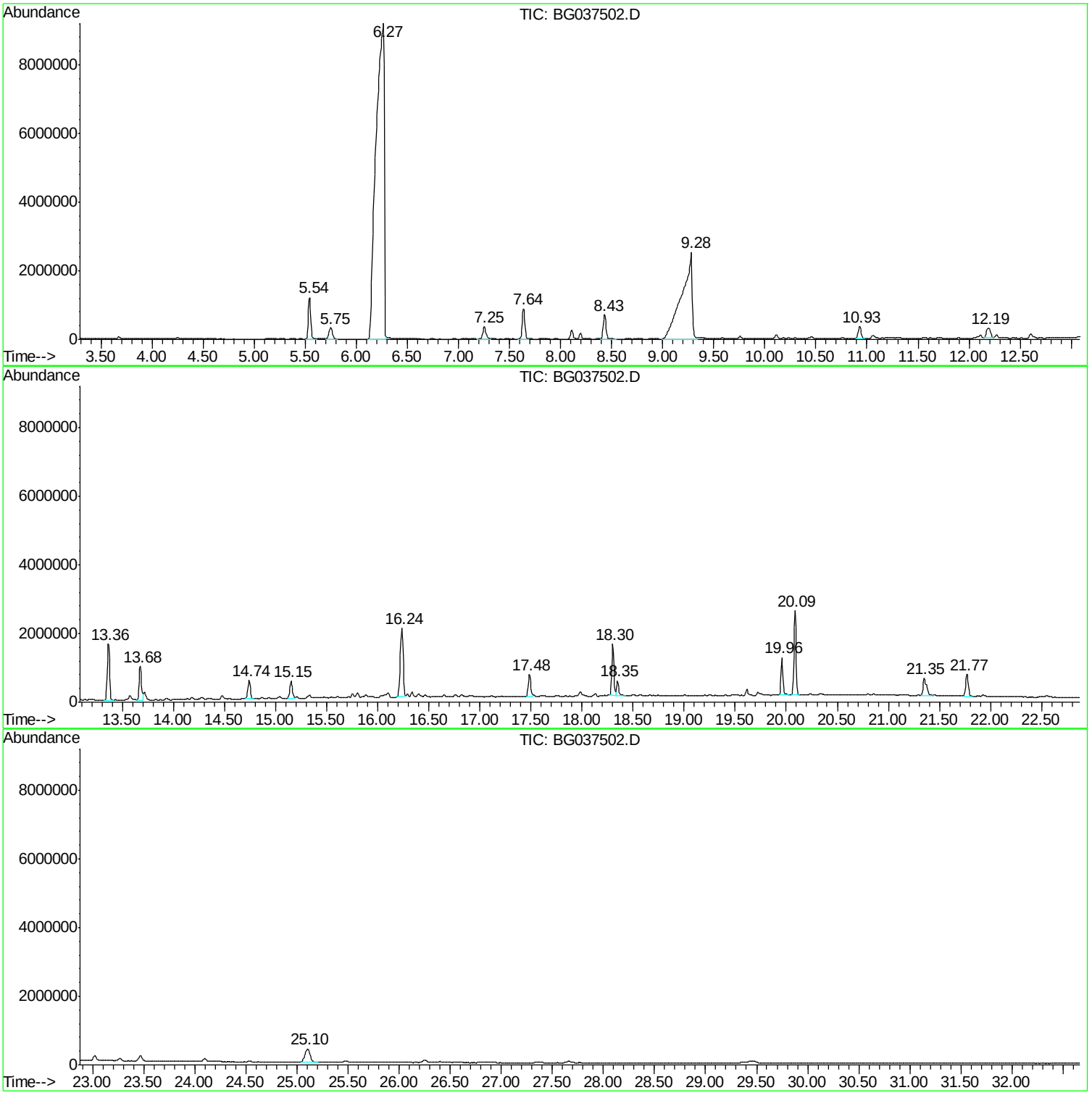
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037502.D
Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

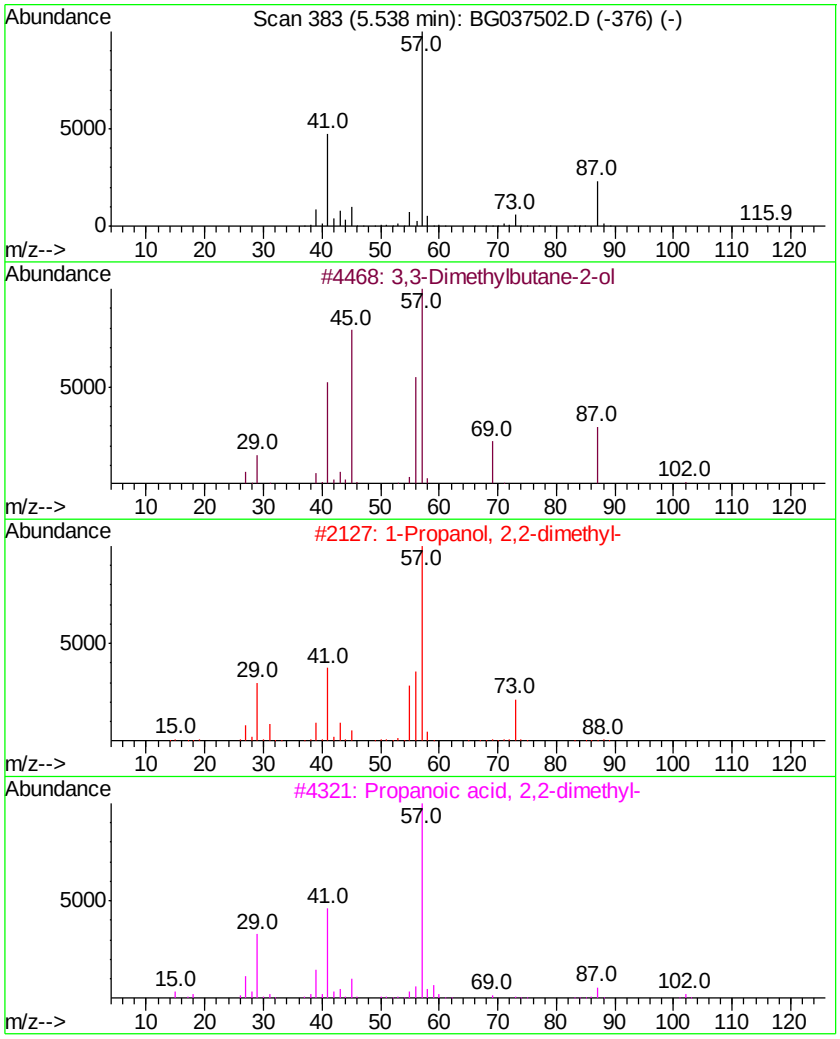
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

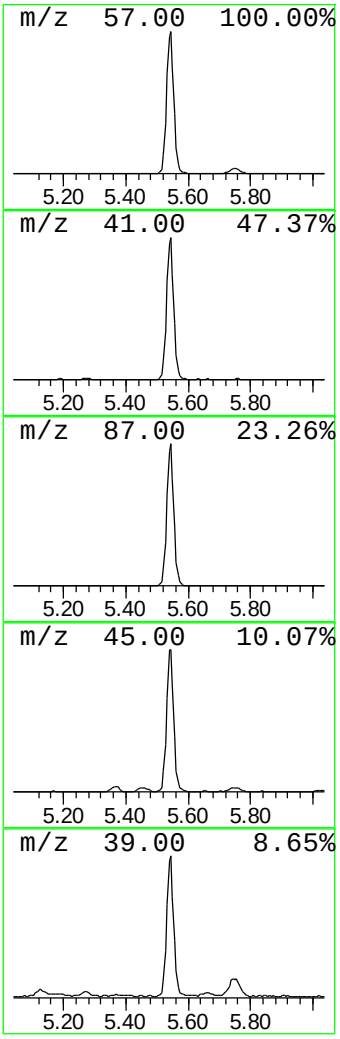
****

Peak Number 1 unknown5.54 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.54	29.33 ng	1993520	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	45
2	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	38
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	38
4	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	36
5	n-Butyl ether	130	C8H18O	000142-96-1	36





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037502.D
Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

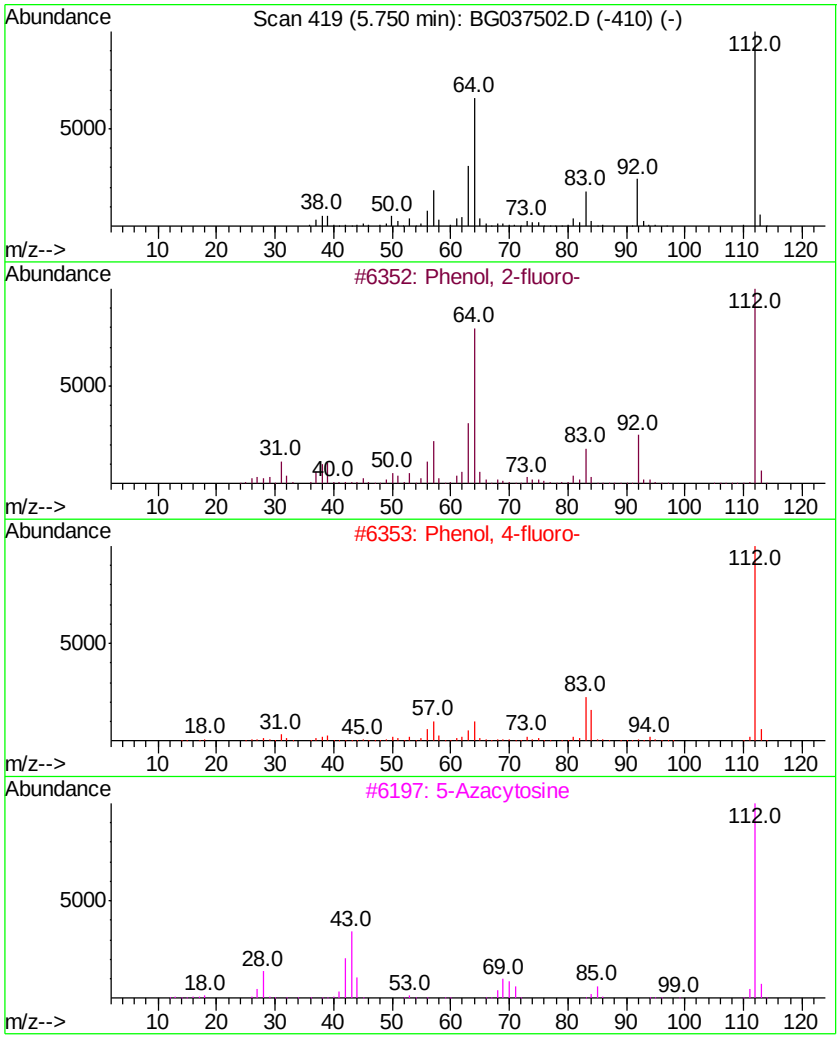
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

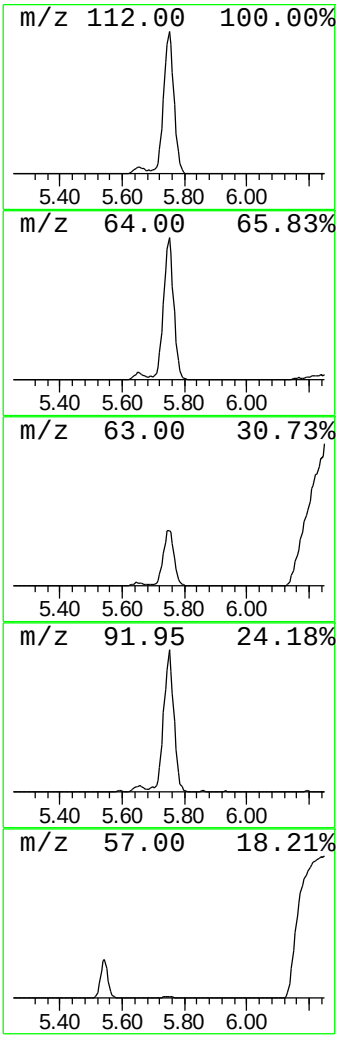
****

Peak Number 2 Phenol, 2-fluoro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.75	11.65 ng	791650	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-fluoro-	112	C6H5FO	000367-12-4	94
2	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	22
3	5-Azacytosine	112	C3H4N4O	000931-86-2	9
4	1H-Tetrazaborole, 4,5-dihydro-1,...	112	C3H9BN4	020546-18-3	9
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037502.D
Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

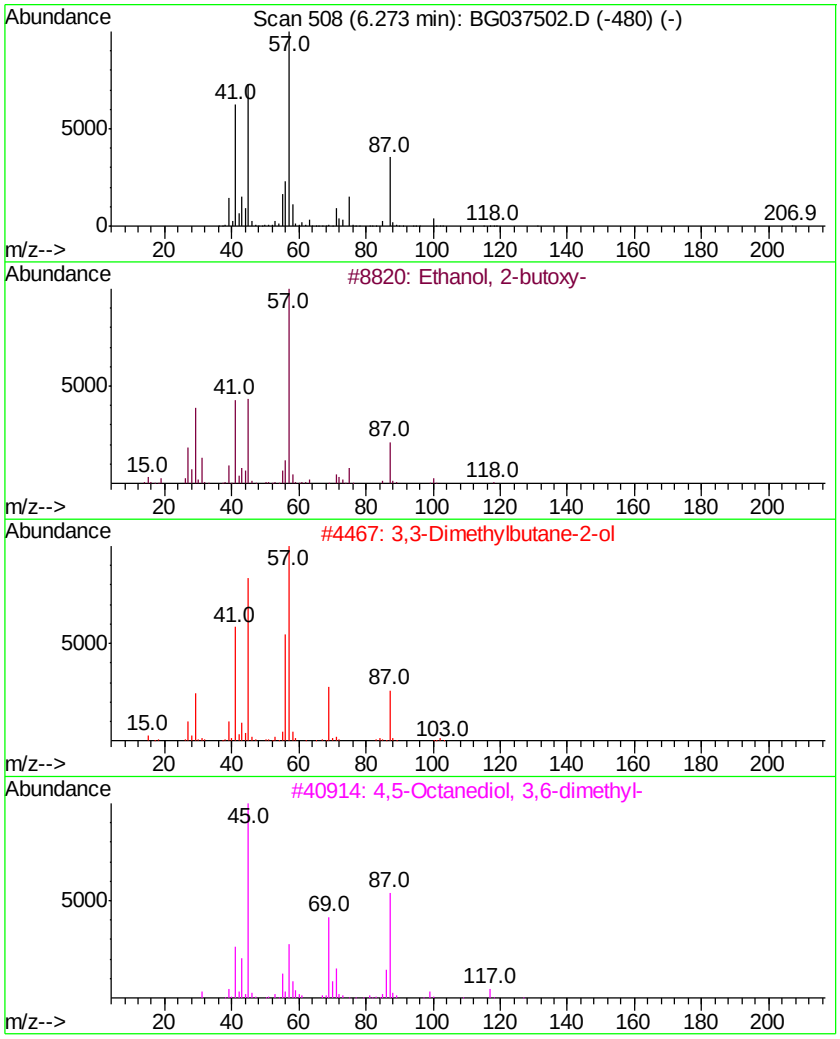
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

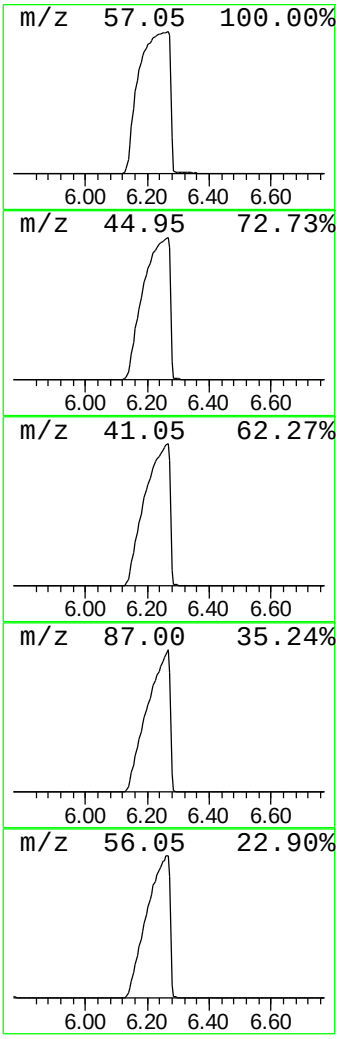
****

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	752.54 ng	51143000	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	72
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
3	4,5-Octanediol, 3,6-dimethyl-	174	C10H22O2	1000153-21-1	38
4	Hexane, 3-methoxy-	116	C7H16O	054658-01-4	33
5	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	33





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037502.D
Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

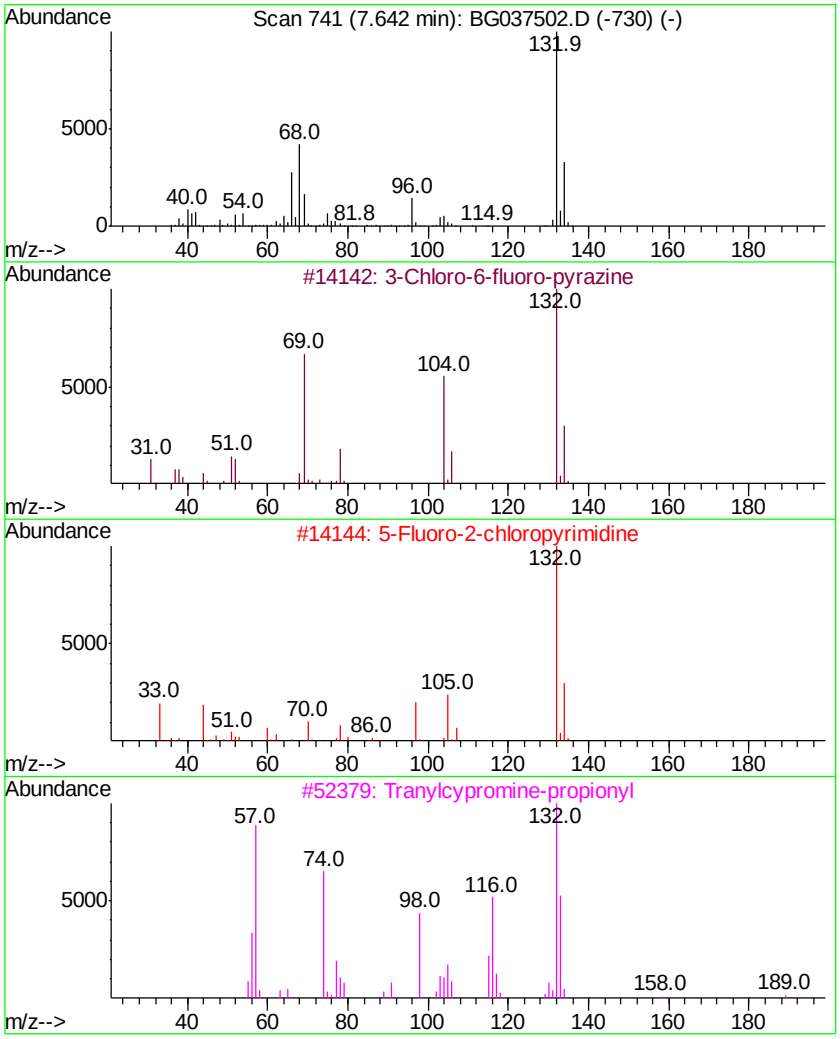
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

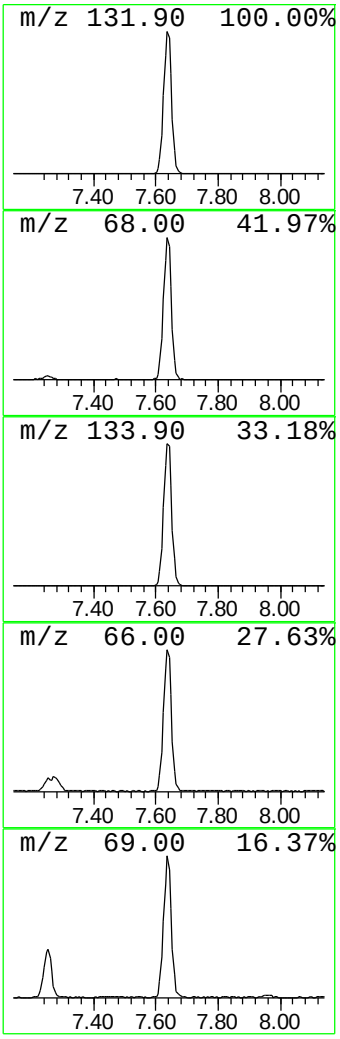
****

Peak Number 4 unknown7.64 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	23.76 ng	1615010	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037502.D
Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

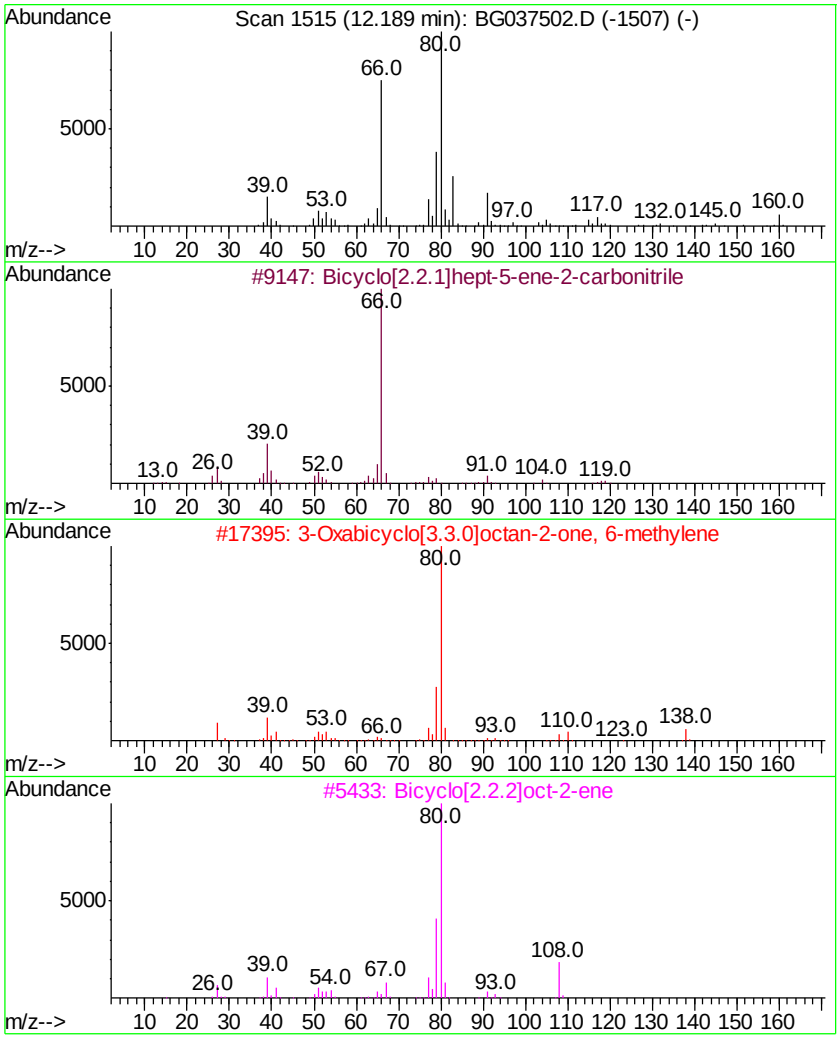
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

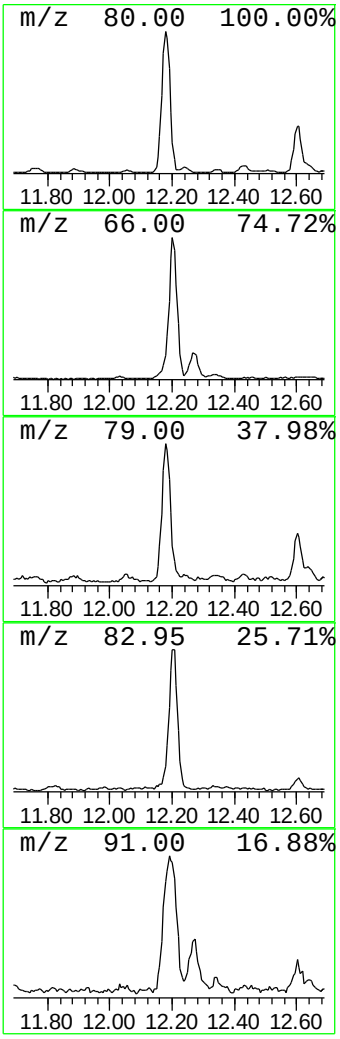
****

Peak Number 6 unknown12.19 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.19	24.88 ng	811302	Naphthalene-d8	10.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]hept-5-ene-2-carbo...	119	C8H9N	000095-11-4	41
2	3-Oxabicyclo[3.3.0]octan-2-one, ...	138	C8H10O2	1000152-82-0	38
3	Bicyclo[2.2.2]oct-2-ene	108	C8H12	000931-64-6	38
4	Bicyclo[3.2.0]hept-2-ene, 2-methyl-	108	C8H12	094122-58-4	38
5	Bicyclo[2.2.1]hept-2-ene, 1-methyl-	108	C8H12	000822-73-1	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037502.D
Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

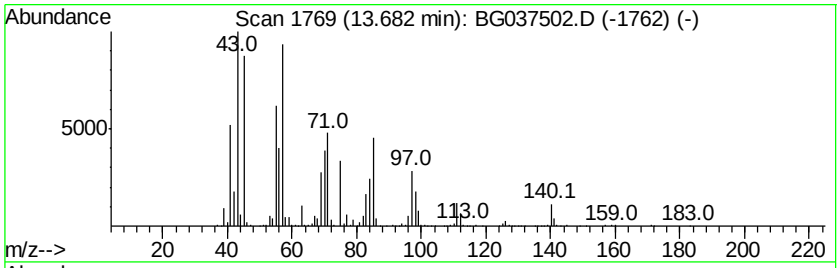
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

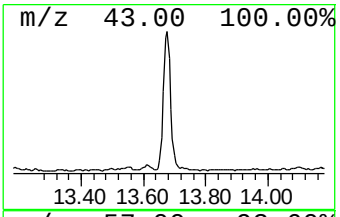
****

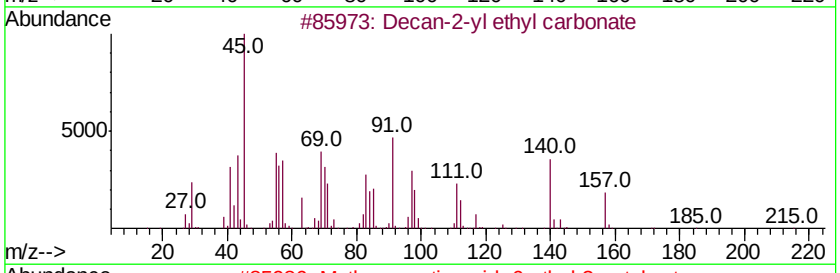
Peak Number 7 unknown13.68 Concentration Rank 3

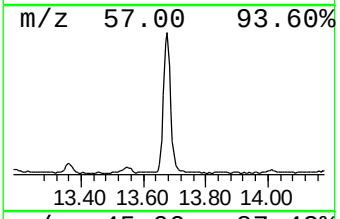
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	35.08 ng	1556600	Acenaphthene-d10	14.74

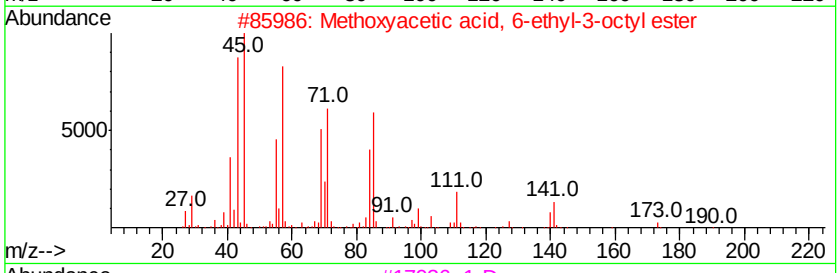
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decan-2-yl ethyl carbonate	230	C13H26O3	1000373-78-9	47
2	Methoxyacetic acid, 6-ethyl-3-oc...	230	C13H26O3	1000282-69-8	47
3	1-Decene	140	C10H20	000872-05-9	46
4	Decane, 1-fluoro-	160	C10H21F	000334-56-5	46
5	Cyclodecane	140	C10H20	000293-96-9	41

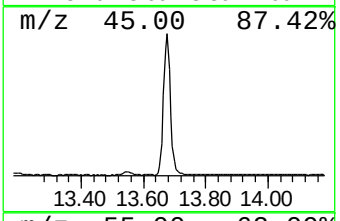


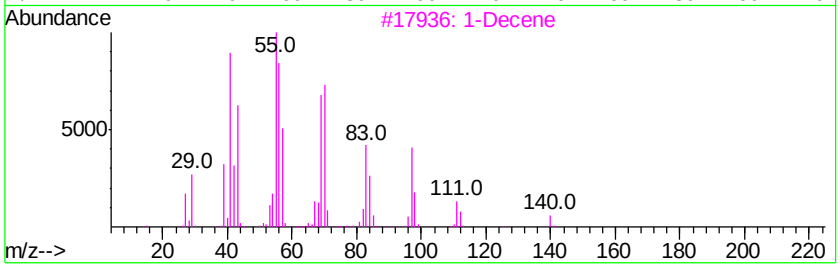


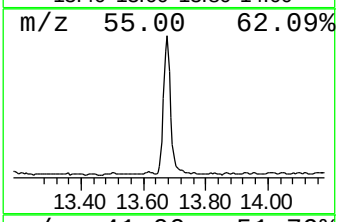


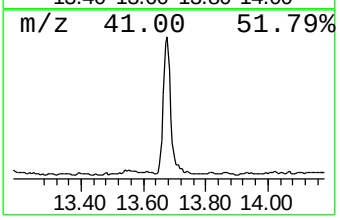












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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

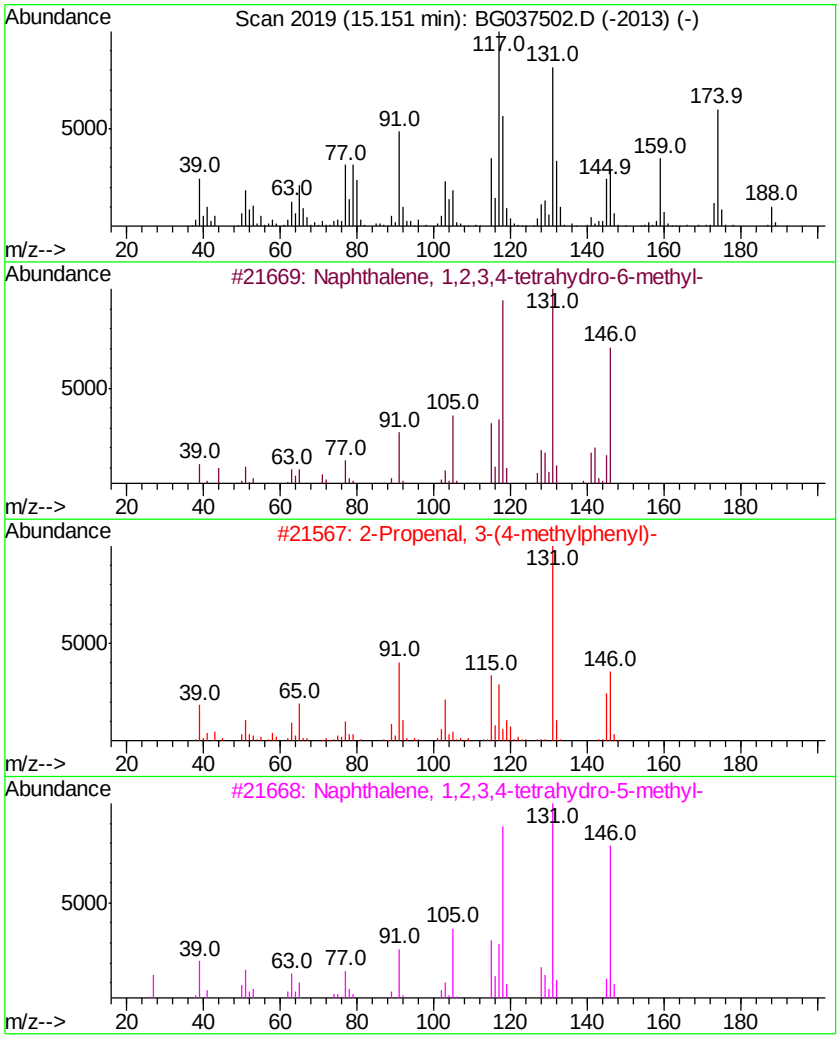
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

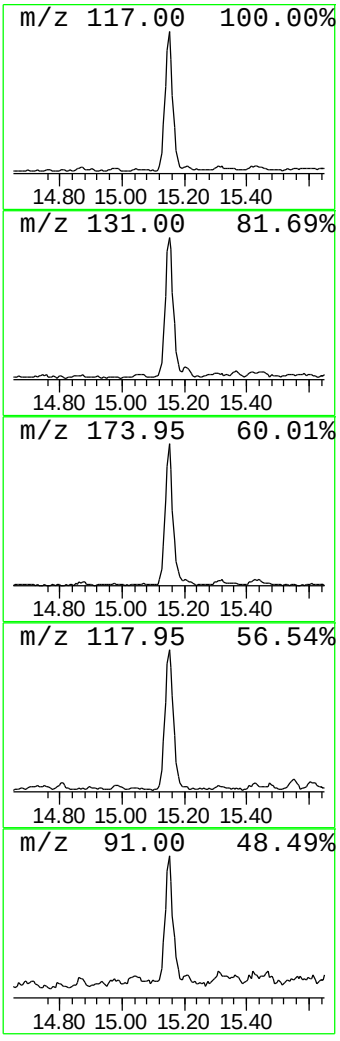
****

Peak Number 8 unknown15.15 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	20.31 ng	900984	Acenaphthene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	46
2	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	46
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	46
4	Azulene, 1,2,3,3a-tetrahydro-	132	C10H12	033877-87-1	38
5	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	38





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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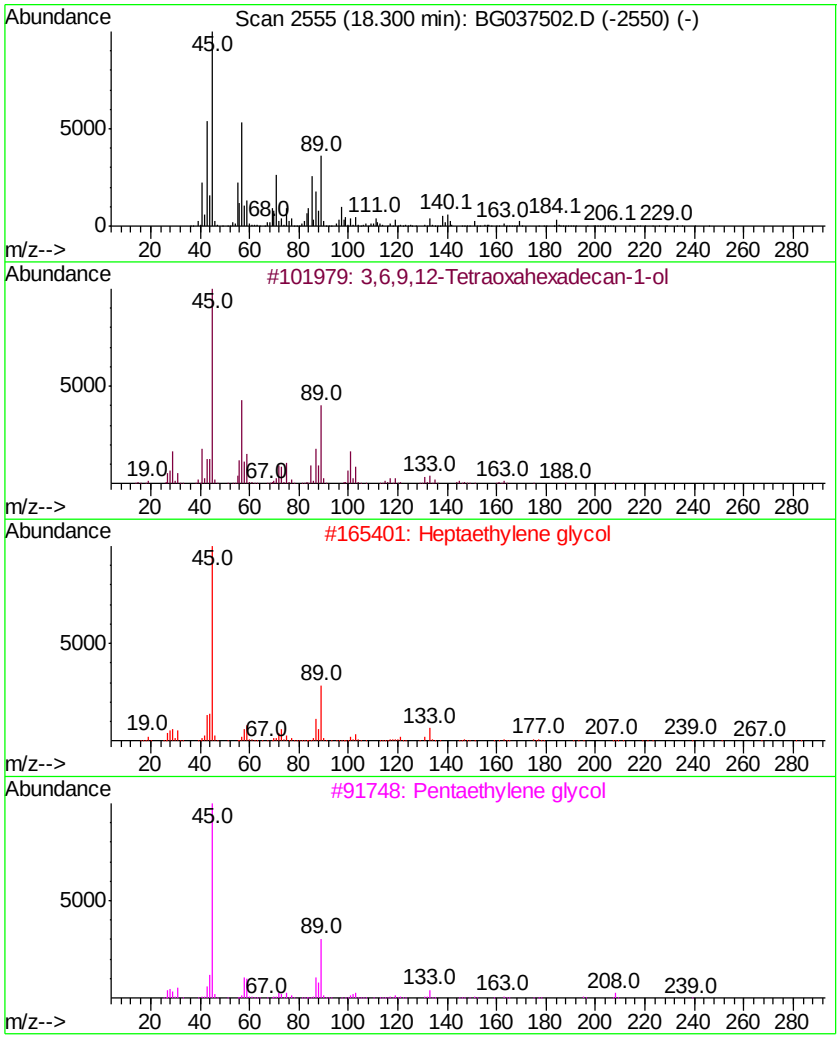
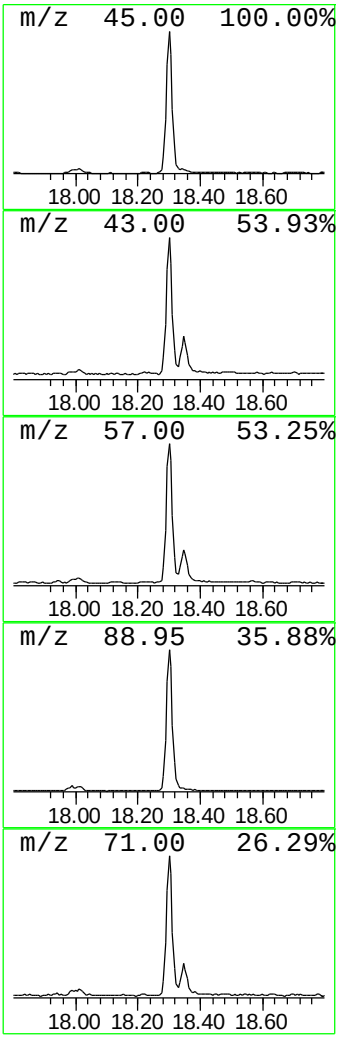
****

Peak Number 9 3,6,9,12-Tetraoxahexadecan-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	39.70 ng	2034340	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	52
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	50
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	50
4	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	50
5	Tetraethyleneglycol monomethylether	208	C9H20O5	023783-42-8	47





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Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

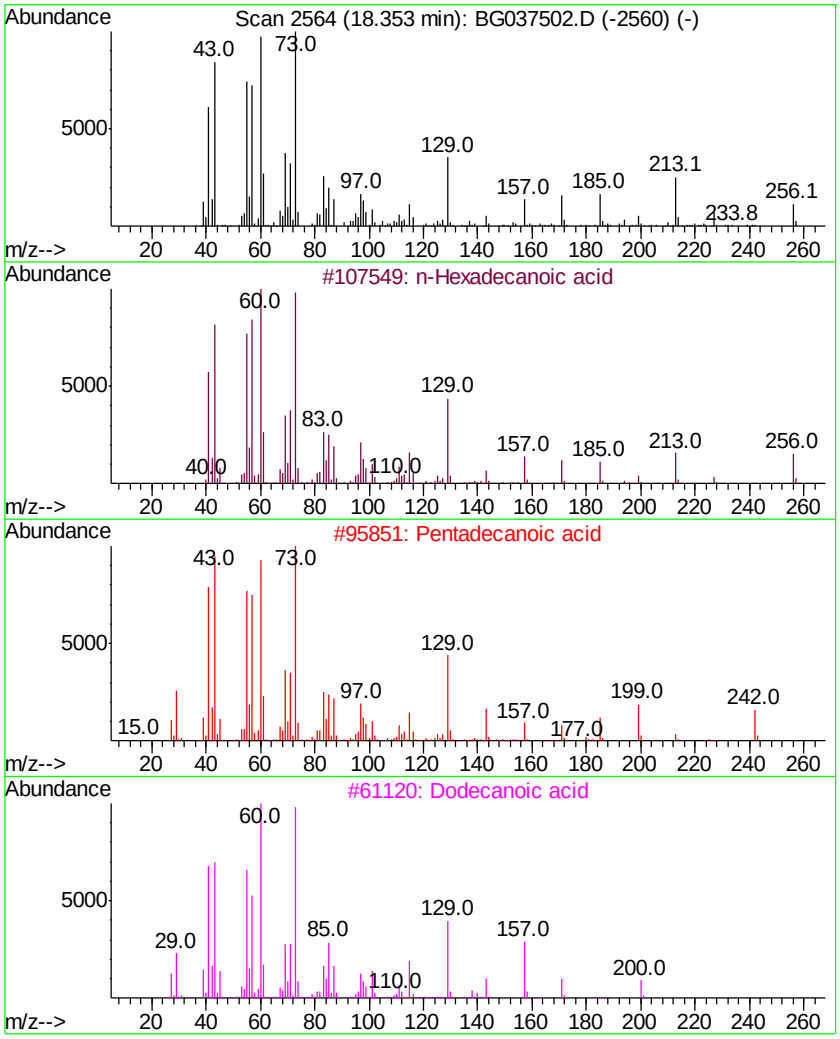
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

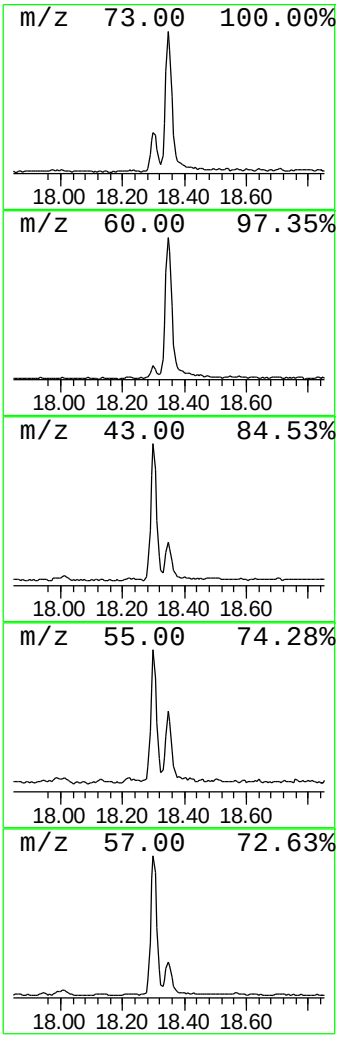
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	12.20 ng	625063	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Dodecanoic acid	200	C12H24O2	000143-07-7	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037502.D
Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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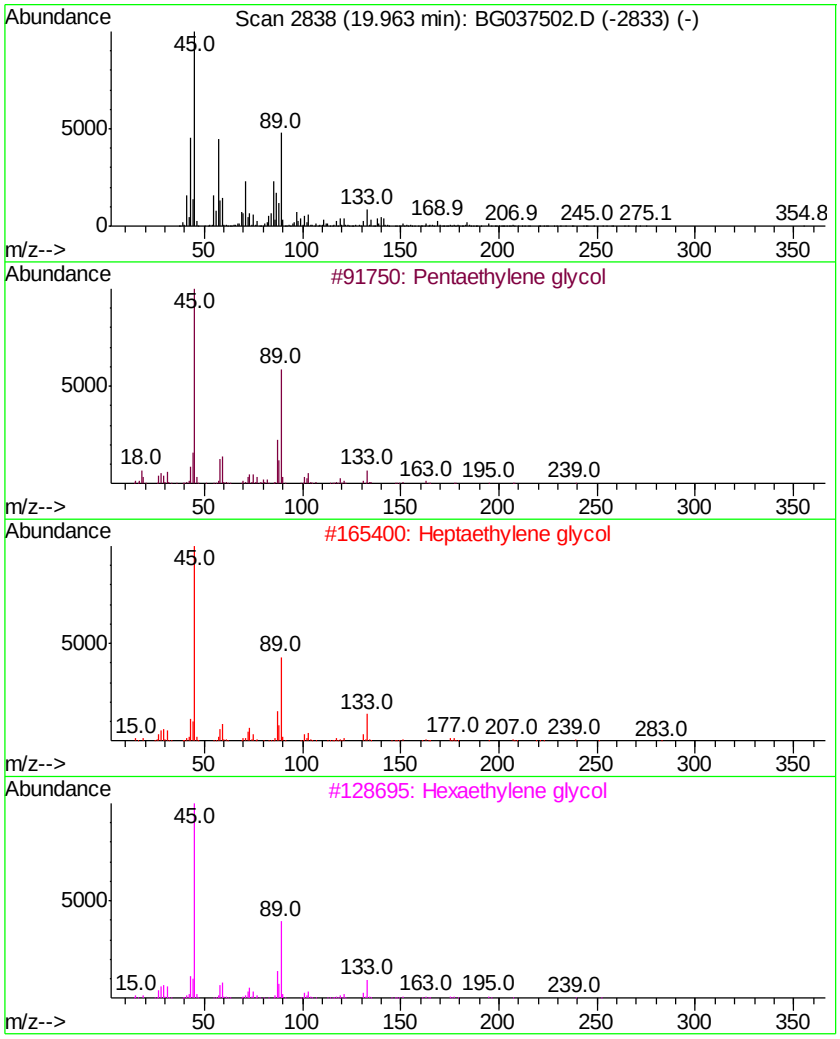
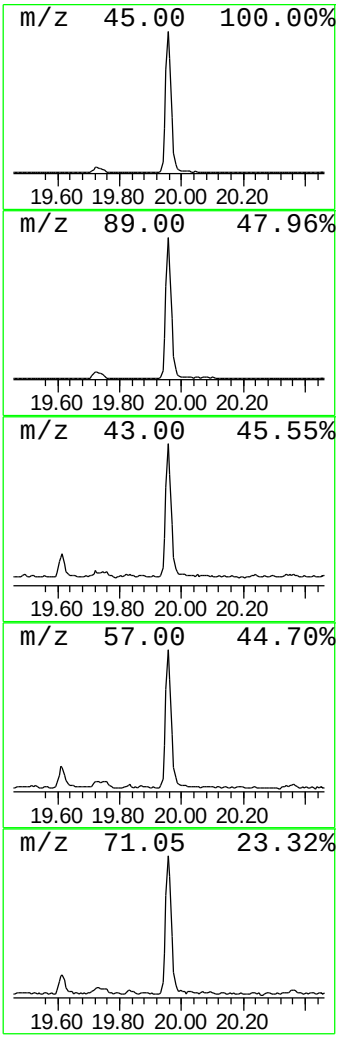
Peak Number 11 Pentaethylene glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.96	25.16 ng	1389690	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	68
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	64
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	64
4	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	64
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102318\
Data File : BG037502.D
Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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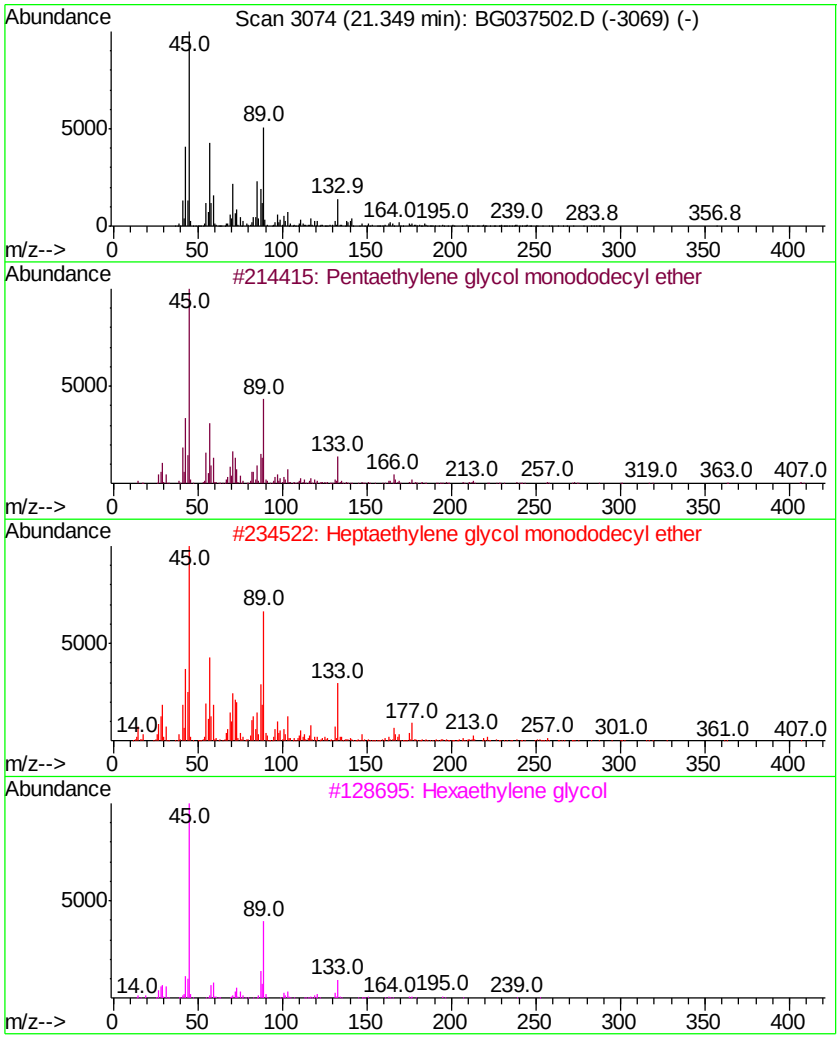
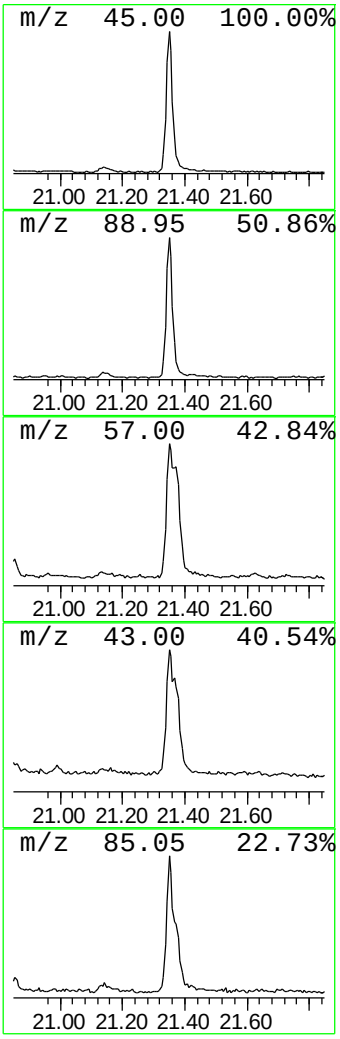
Peak Number 12 Pentaethylene glycol monodo... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	20.28 ng	1120130	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	86
2	Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	78
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	68
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	68
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102318\
Data File : BG037502.D
Acq On : 24 Oct 2018 8:58
Operator : JU/SJ
Sample : J5604-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MS-VB-29736-BOX-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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
unknown5.54	5.54	29.3	ng	1993520	1	8.11	1359210	20.0
Phenol, 2-fluoro-	5.75	11.7	ng	791650	1	8.11	1359210	20.0
Ethanol, 2-butoxy-	6.27	752.5	ng	51143000	1	8.11	1359210	20.0
unknown7.64	7.64	23.8	ng	1615010	1	8.11	1359210	20.0
unknown12.19	12.19	24.9	ng	811302	2	10.93	652189	20.0
unknown13.68	13.68	35.1	ng	1556600	3	14.74	887361	20.0
unknown15.15	15.15	20.3	ng	900984	3	14.74	887361	20.0
3,6,9,12-Tetraoxa...	18.30	39.7	ng	2034340	4	17.48	1024850	20.0
n-Hexadecanoic acid	18.35	12.2	ng	625063	4	17.48	1024850	20.0
Pentaethylene glycol	19.96	25.2	ng	1389690	5	21.77	1104540	20.0
Pentaethylene gly...	21.35	20.3	ng	1120130	5	21.77	1104540	20.0