LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062718\
Data File : BG035458.D
Acq On : 27 Jun 2018 23:25
Operator : JU/SJ
Sample : J3694-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-4

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-BG060718.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	5.163	314	319	328	rBV	33571	53260	1.05%	0.240%
2	5.627	390	398	410	rBV	443507	749978	14.81%	3.375%
3	7.213	658	668	681	rBV	285074	534328	10.56%	2.404%
4	7.583	724	731	741	rBV	863983	1508725	29.80%	6.789%
5	8.053	804	811	818	rBV	174503	302334	5.97%	1.360%
6	8.376	859	866	875	rVB	691383	1200714	23.72%	5.403%
7	9.210	998	1008	1024	rBV	661307	1224085	24.18%	5.508%
8	10.855	1281	1288	1297	rBV	229198	401228	7.93%	1.805%
9	13.299	1694	1704	1713	rBV	1806118	2759972	54.52%	12.419%
10	14.121	1836	1844	1850	rBV2	56597	89463	1.77%	0.403%
11	14.673	1931	1938	1943	rBV2	395701	661878	13.07%	2.978%
12	14.720	1943	1946	1952	rVV2	51479	78411	1.55%	0.353%
13	16.160	2183	2191	2200	rBV	1691553	2593967	51.24%	11.672%
14	17.417	2398	2405	2411	rBV	544122	810320	16.01%	3.646%
15	18.298	2550	2555	2562	rBV	78940	129311	2.55%	0.582%
16	18.386	2565	2570	2578	rVV2	96542	174575	3.45%	0.786%
17	18.515	2587	2592	2600	rBV	63701	105019	2.07%	0.473%
18	19.643	2779	2784	2792	rBV	248183	391711	7.74%	1.763%
19	20.025	2843	2849	2863	rBV	3519126	5062307	100.00%	22.778%
20	20.266	2885	2890	2896	rVB	79589	107131	2.12%	0.482%
21	20.894	2991	2997	3003	rBV	122820	167789	3.31%	0.755%
22	21.335	3067	3072	3080	rBV7	49950	105465	2.08%	0.475%
23	21.435	3084	3089	3103	rBV	249717	463260	9.15%	2.084%
24	21.681	3125	3131	3140	rVB	591129	986061	19.48%	4.437%
25	23.132	3372	3378	3387	rBV2	161300	383083	7.57%	1.724%
26	24.901	3669	3679	3692	rVB2	324670	922241	18.22%	4.150%
27	25.635	3793	3804	3814	rBV3	70140	257990	5.10%	1.161%

Sum of corrected areas: 22224606

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062718\
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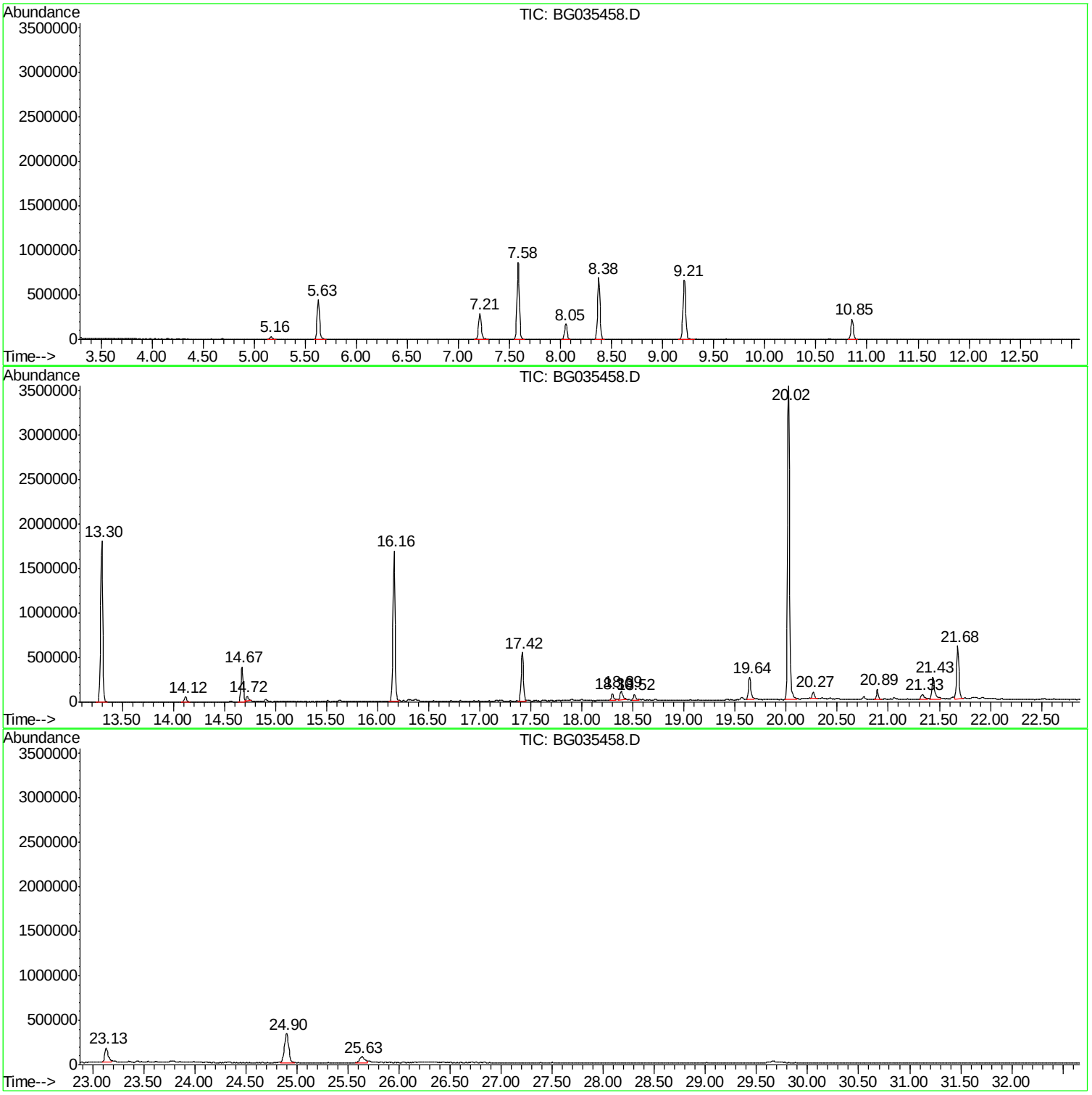
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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 : BG035458.D
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Operator : JU/SJ
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Misc :
ALS Vial : 14 Sample Multiplier: 1

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ClientSampleId : PZ-4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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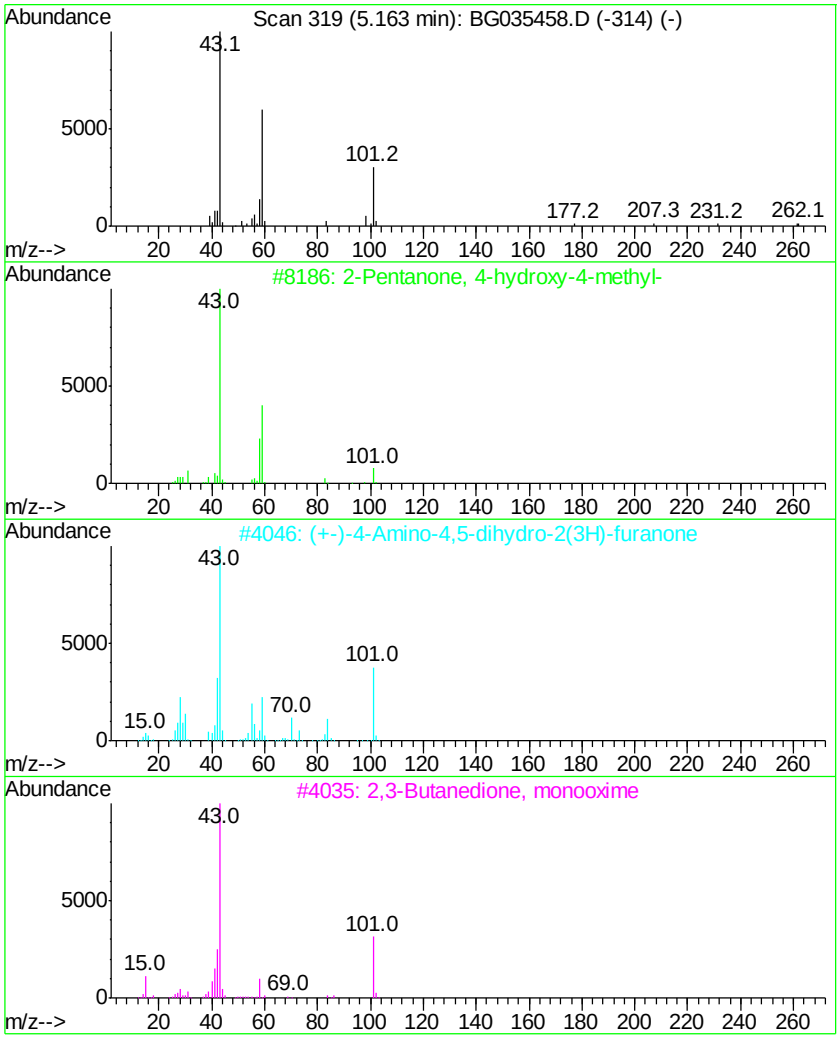
TIC Integration Parameters: LSCINT.P

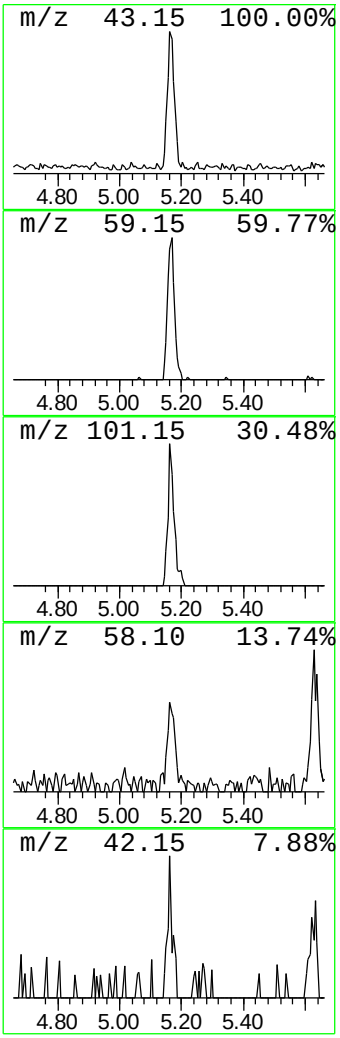
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	3.52 ng	53260	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	23
5	3-Heptadecanol	256	C17H36O	084534-30-5	17





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Operator : JU/SJ
Sample : J3694-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

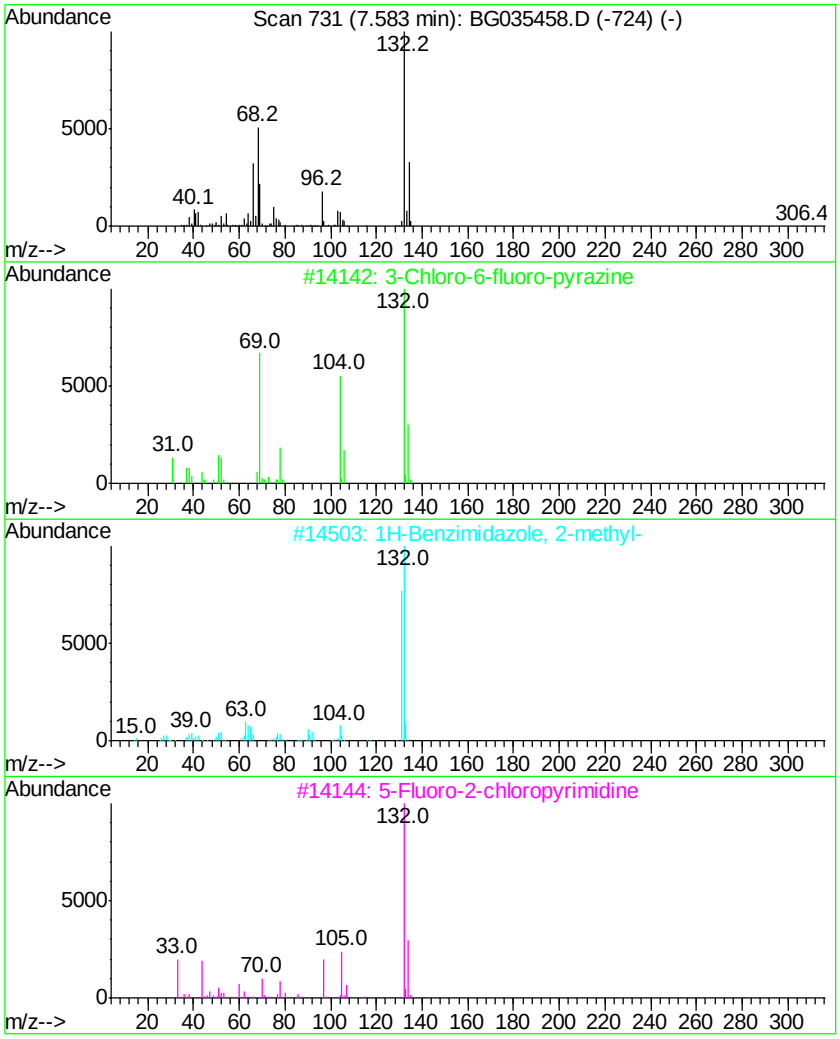
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

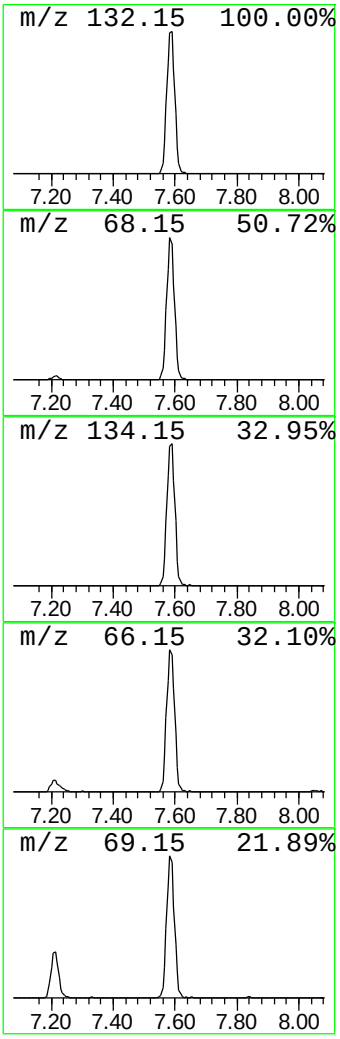
****

Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	99.81 ng	1508730	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062718\
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Acq On : 27 Jun 2018 23:25
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Sample : J3694-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

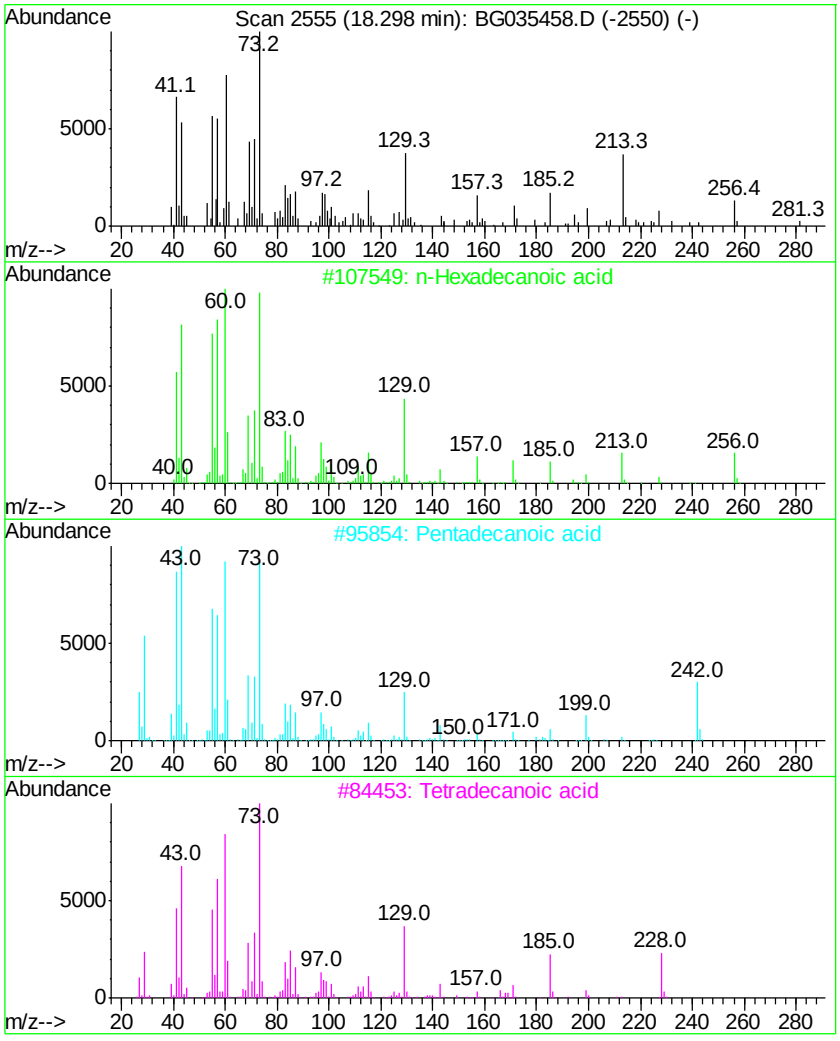
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

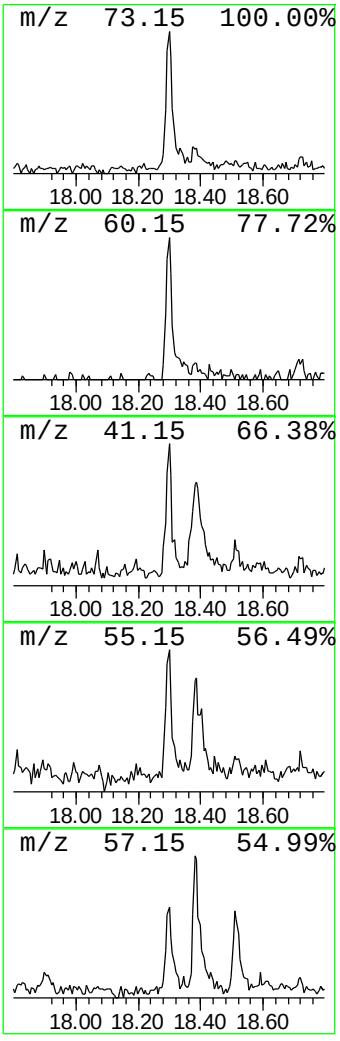
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.19 ng	129311	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	52
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062718\
Data File : BG035458.D
Acq On : 27 Jun 2018 23:25
Operator : JU/SJ
Sample : J3694-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

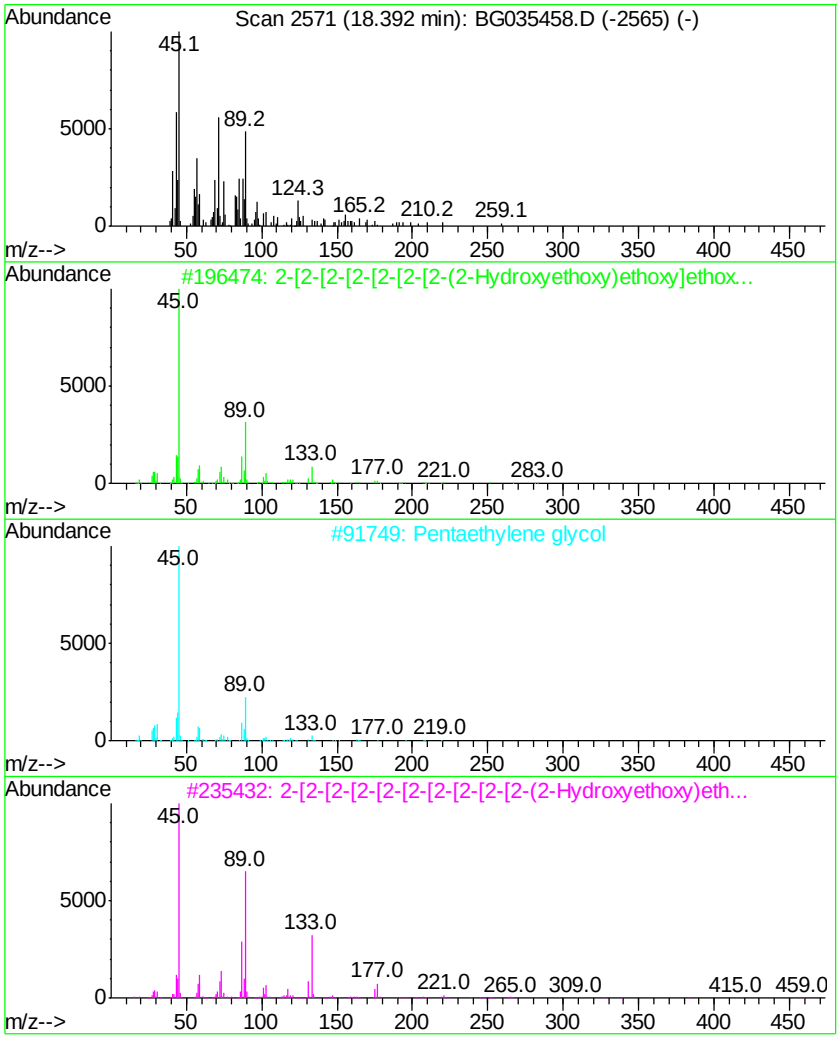
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

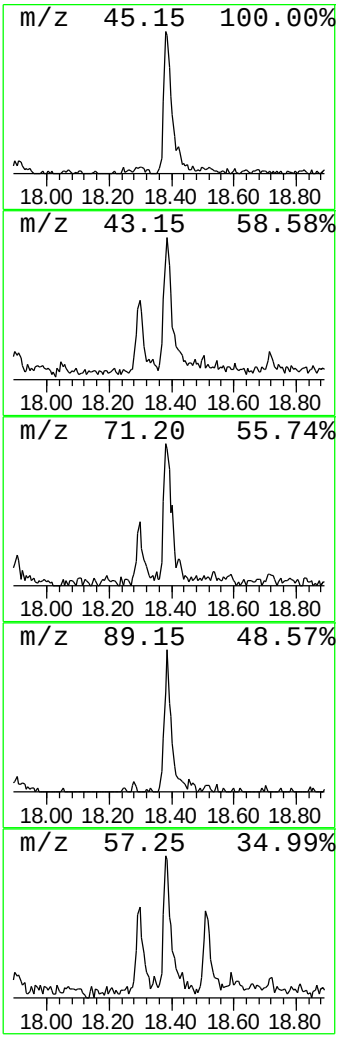
****

Peak Number 5 unknown18.39 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	4.31 ng	174575	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	47
2	Pentaethylene glycol	238	C10H22O6	004792-15-8	38
3	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	38
4	Cyclohexyl-15-crown-5	274	C14H26O5	017454-48-7	38
5	2-Propanol, 1,1'-oxybis-	134	C6H14O3	000110-98-5	35





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Operator : JU/SJ
Sample : J3694-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

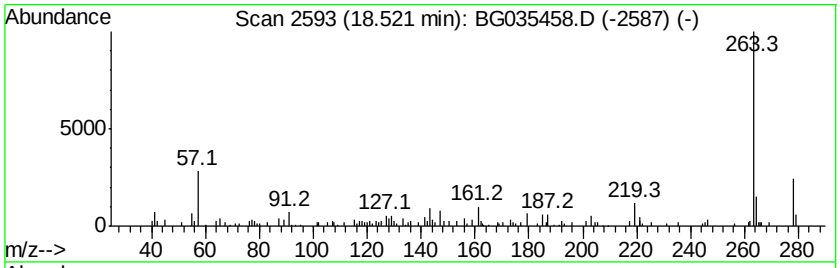
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

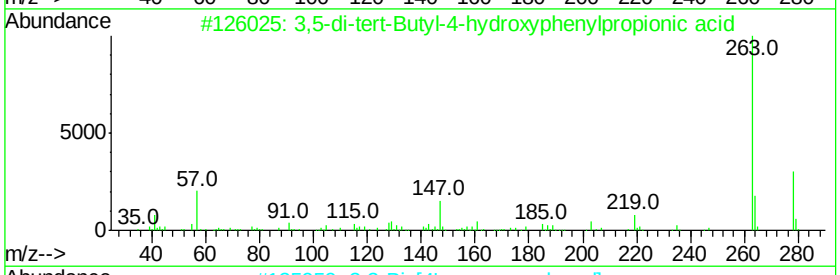
****

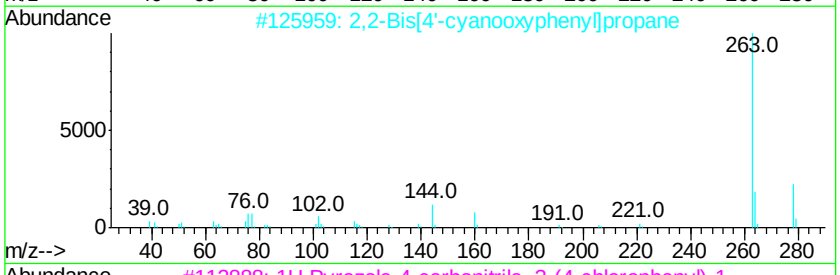
Peak Number 6 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 10

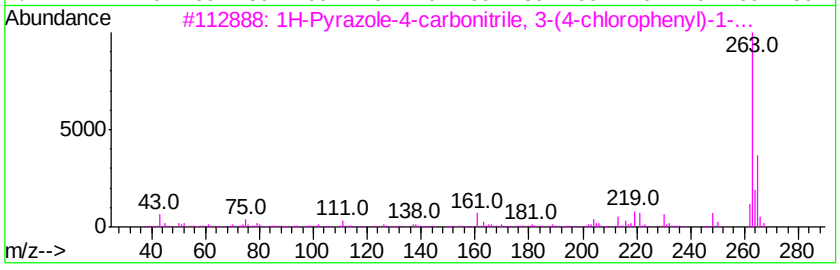
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.52	2.59 ng	105019	Phenanthrene-d10	17.42

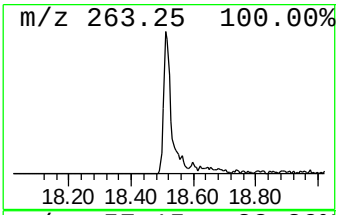
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxyphenyl...	278	C17H26O3	020170-32-5	94
2	2,2-Bis[4'-cyanooxyphenyl]propane	278	C17H14N2O2	1000322-13-3	74
3	1H-Pyrazole-4-carbonitrile, 3-(4...	263	C12H10ClN3S	068364-67-0	53
4	7-Methyl-2-phenylquinoline-4-car...	263	C17H13NO2	181048-54-4	53
5	1-(6-Amino-8-morpholin-4-yl-puri...	363	C16H25N7O3	1000294-67-5	50

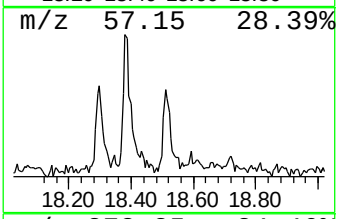


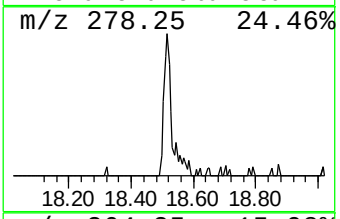


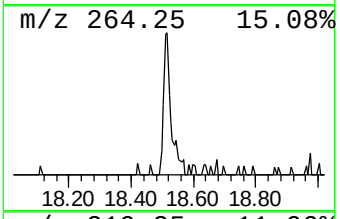


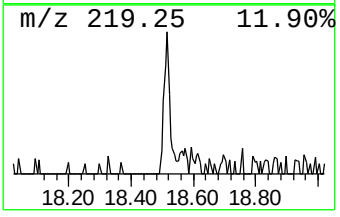












Library Search Compound Report

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Data File : BG035458.D
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

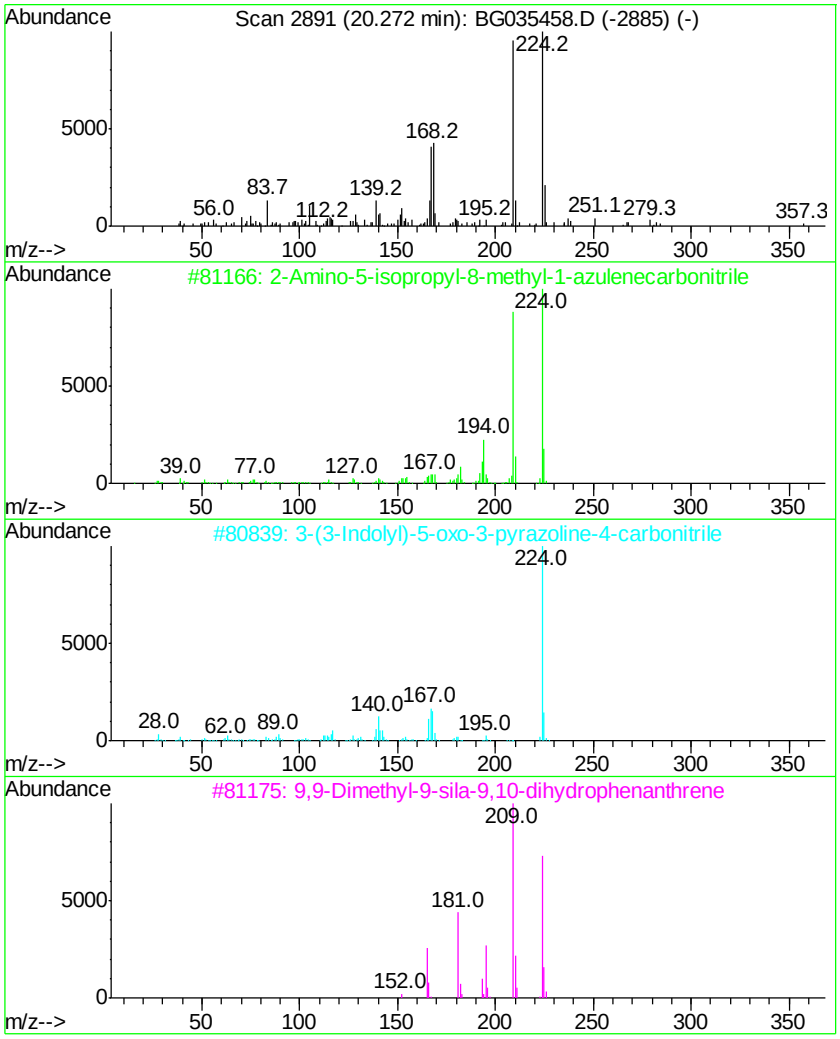
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

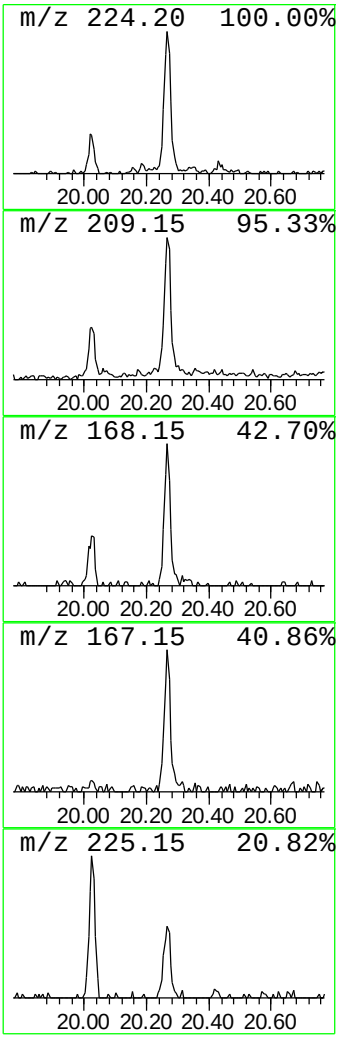
****

Peak Number 7 2-Amino-5-isopropyl-8-methy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.27	2.17 ng	107131	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-5-isopropyl-8-methyl-1-a...	224	C15H16N2	093946-48-6	52
2	3-(3-Indolyl)-5-oxo-3-pyrazoline...	224	C12H8N4O	1000240-73-4	46
3	9,9-Dimethyl-9-sila-9,10-dihydro...	224	C15H16Si	187328-55-8	43
4	Dibenzo[d,f]-1,3,2-dioxaborepine...	224	C14H13BO2	1000160-51-1	38
5	1,3,6,9b-Tetraazaphenalene-4-car...	209	C11H7N5	037160-08-0	38





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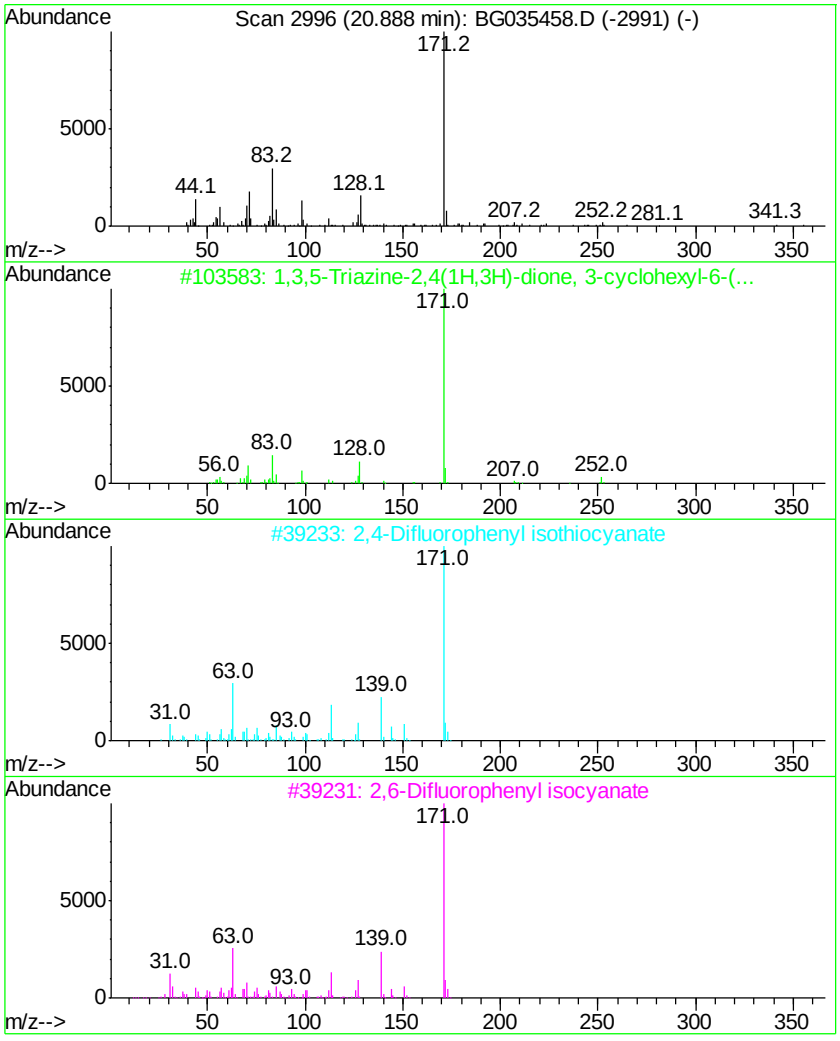
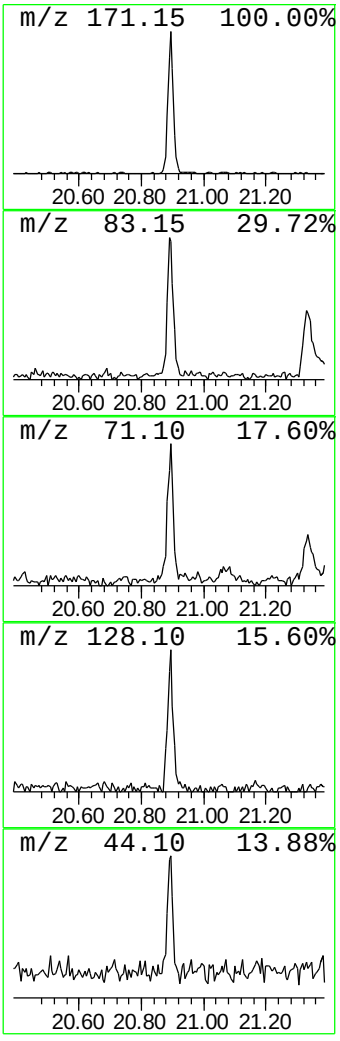
****

Peak Number 8 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.89	3.40 ng	167789	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	94
2	2,4-Difluorophenyl isothiocyanate	171	C7H3F2NS	141106-52-7	40
3	2,6-Difluorophenyl isocyanate	171	C7H3F2NS	065295-69-4	40
4	Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FNO2	1000116-43-3	38
5	Pyrimidine-2,4,6(1H,3H,5H)-trion...	334	C17H26N4O3	201928-46-3	17





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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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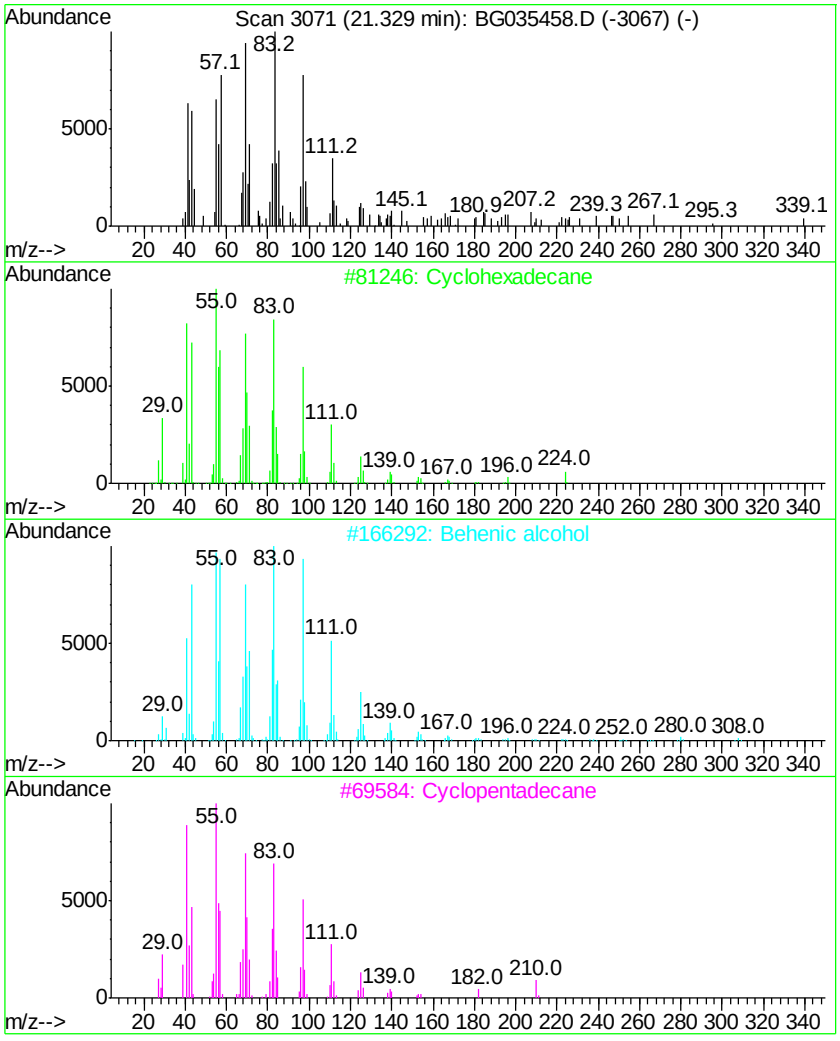
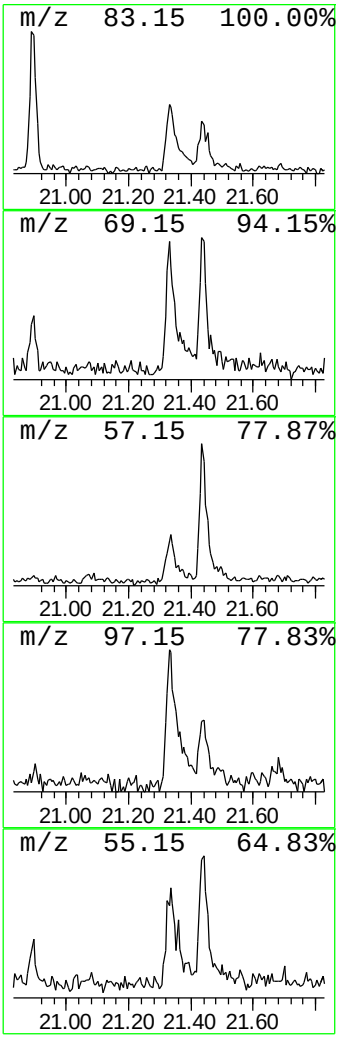
****

Peak Number 9 Cyclohexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	2.14 ng	105465	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	97
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Cyclopentadecane	210	C15H30	000295-48-7	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	1-Heptacosanol	396	C27H56O	002004-39-9	93





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062718\
Data File : BG035458.D
Acq On : 27 Jun 2018 23:25
Operator : JU/SJ
Sample : J3694-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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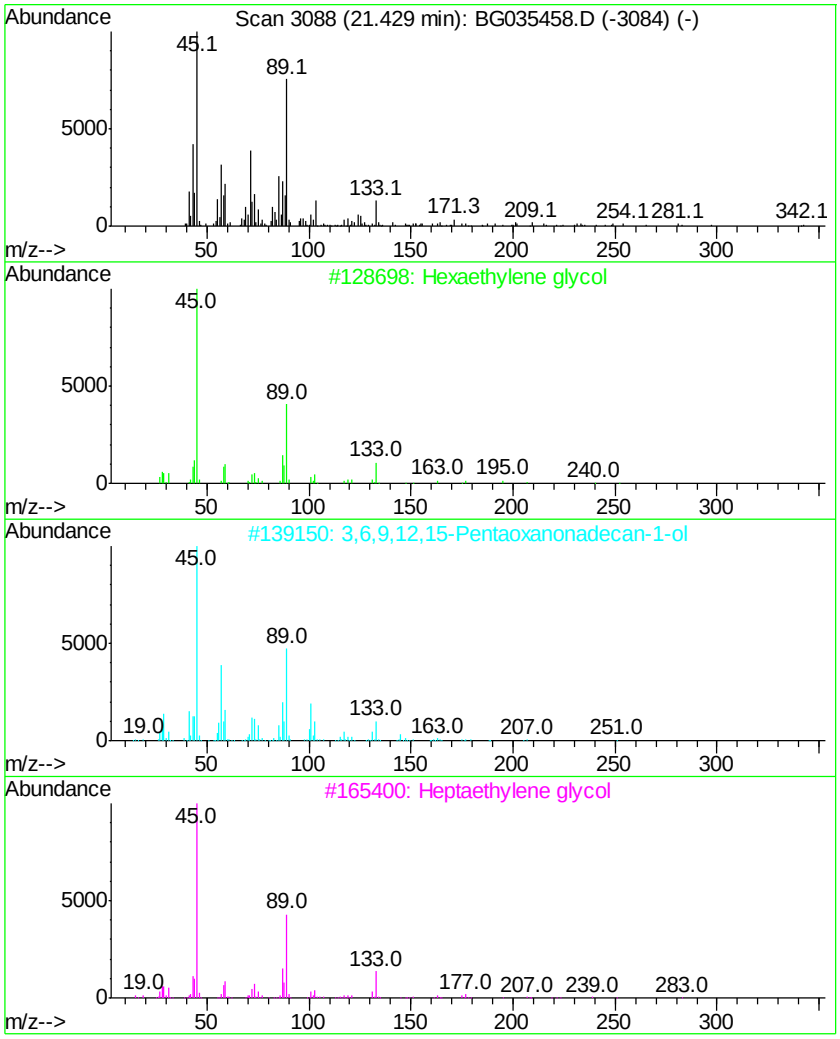
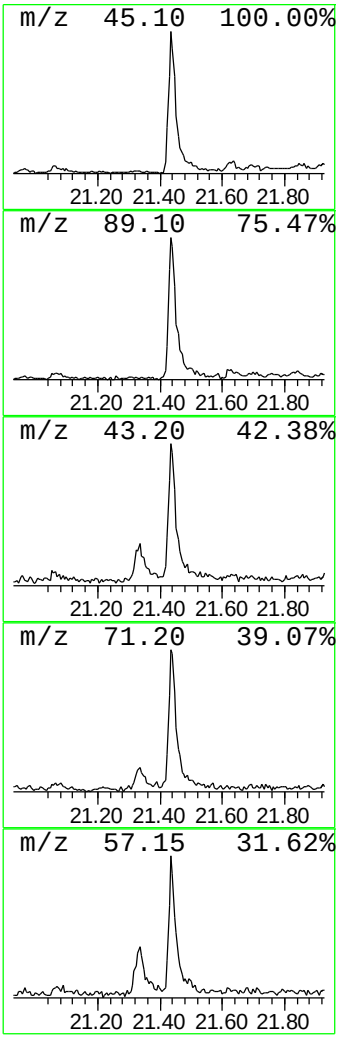
Peak Number 10 Hexaethylene glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.43	9.40 ng	463260	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	64
2	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	64
3	Heptaethylene glycol	326	C14H30O8	005617-32-3	58
4	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	58
5	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	58





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Data File : BG035458.D
Acq On : 27 Jun 2018 23:25
Operator : JU/SJ
Sample : J3694-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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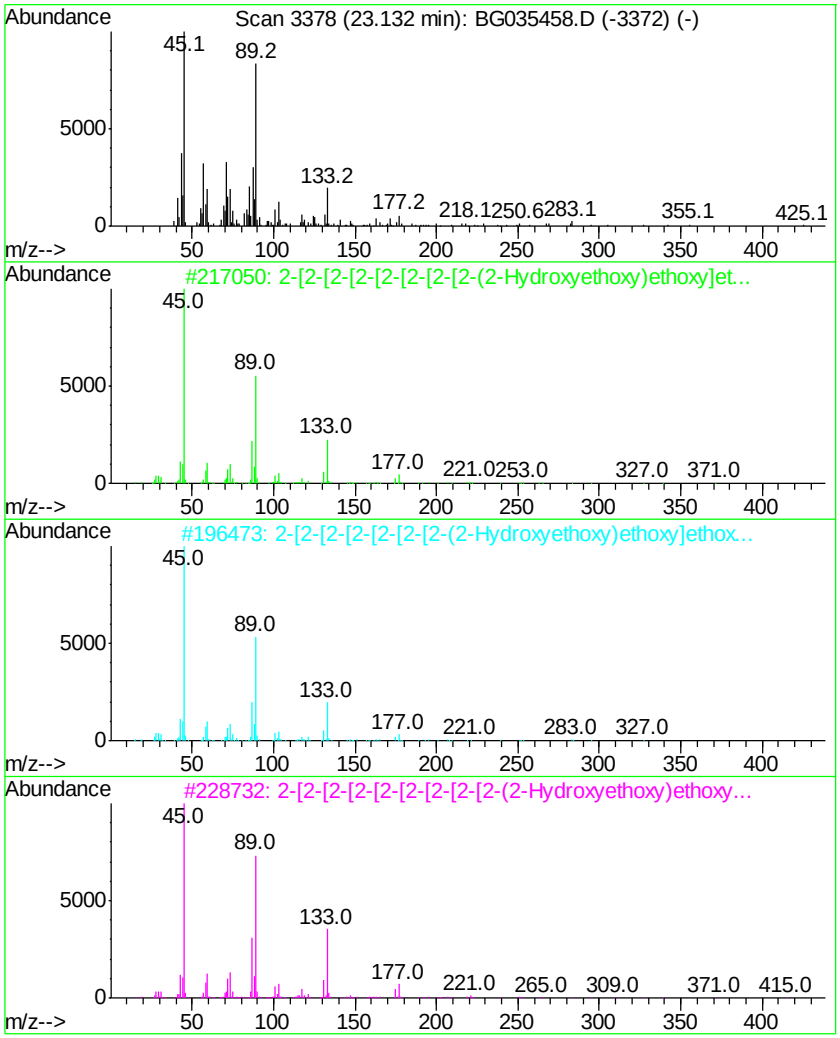
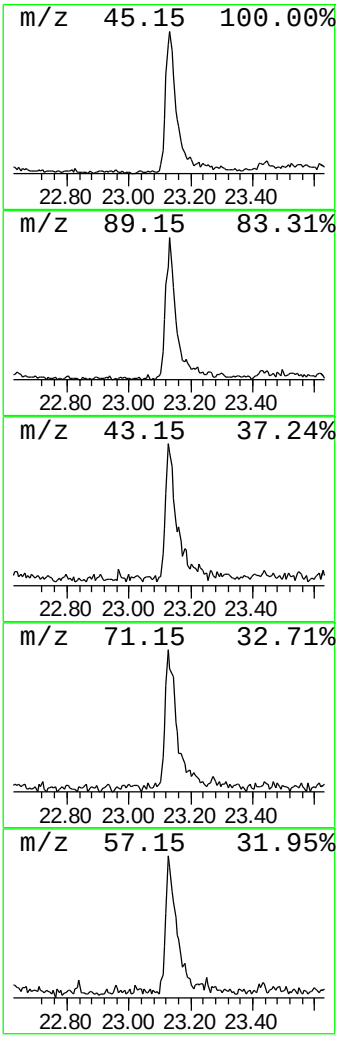
Peak Number 11 2-[2-[2-[2-[2-[2-[2-[2-(2-H... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.13	7.77 ng	383083	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	91
2	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	90
3	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	86
4	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	86
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062718\
Data File : BG035458.D
Acq On : 27 Jun 2018 23:25
Operator : JU/SJ
Sample : J3694-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PZ-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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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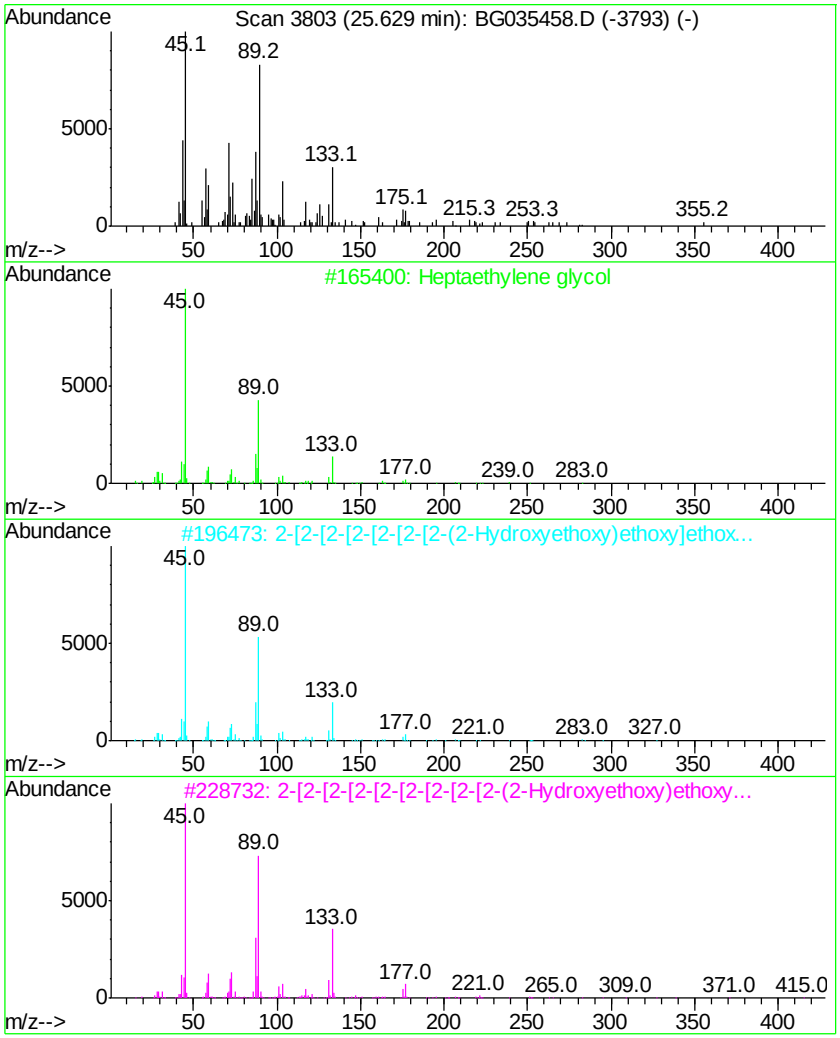
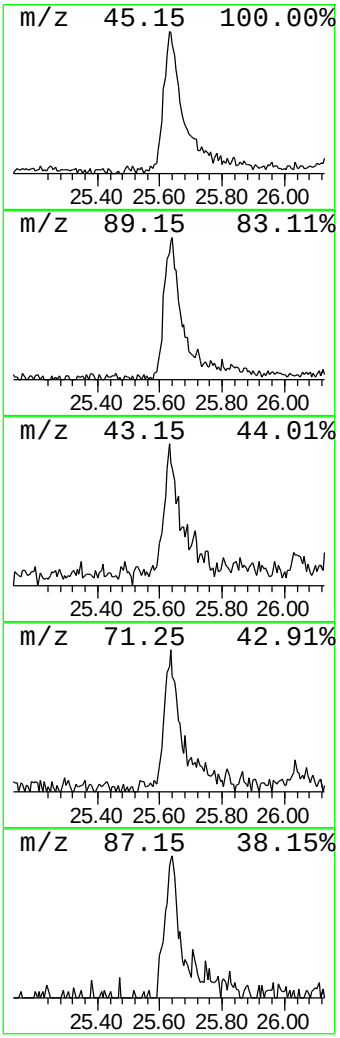
Peak Number 12 Heptaethylene glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.63	5.59 ng	257990	Perylene-d12	24.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	74
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	74
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	72
4	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	72
5	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG062718\
Data File : BG035458.D
Acq On : 27 Jun 2018 23:25
Operator : JU/SJ
Sample : J3694-01
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Instrument : BNA_G
ClientSampleId : PZ-4

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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
2-Pentanone, 4-hy...	5.16	3.5	ng	53260	1	8.05	302334	20.0
unknown7.58	7.58	99.8	ng	1508730	1	8.05	302334	20.0
n-Hexadecanoic acid	18.30	3.2	ng	129311	4	17.42	810320	20.0
unknown18.39	18.39	4.3	ng	174575	4	17.42	810320	20.0
3,5-di-tert-Butyl...	18.52	2.6	ng	105019	4	17.42	810320	20.0
2-Amino-5-isoprop...	20.27	2.2	ng	107131	5	21.68	986061	20.0
1,3,5-Triazine-2,...	20.89	3.4	ng	167789	5	21.68	986061	20.0
Cyclohexadecane	21.33	2.1	ng	105465	5	21.68	986061	20.0
Hexaethylene glycol	21.43	9.4	ng	463260	5	21.68	986061	20.0
2-[2-[2-[2-[2-[2-...	23.13	7.8	ng	383083	5	21.68	986061	20.0
Heptaethylene glycol	25.63	5.6	ng	257990	6	24.90	922241	20.0