LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022817\
Data File : BG026001.D
Acq On : 28 Feb 2017 17:39
Operator : SJ/MA
Sample : I2017-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-1-20170227

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-BG021717.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	5.172	305	312	320	rBV	232831	356568	3.24%	0.776%
2	5.642	386	392	404	rVB	969017	1513385	13.77%	3.292%
3	7.228	652	662	673	rBV	616688	1029375	9.36%	2.239%
4	7.610	718	727	737	rBV	1574078	2701811	24.58%	5.877%
5	8.074	799	806	815	rVB	301298	512166	4.66%	1.114%
6	8.403	853	862	871	rVB	1334876	2321253	21.12%	5.049%
7	9.231	994	1003	1013	rBV	1097607	1925986	17.52%	4.190%
8	10.383	1193	1199	1210	rBV	93924	153117	1.39%	0.333%
9	10.877	1274	1283	1291	rBV	480765	835930	7.60%	1.818%
10	13.309	1689	1697	1705	rBV	3602057	5533561	50.34%	12.037%
11	13.644	1748	1754	1762	rBV	222138	326268	2.97%	0.710%
12	14.678	1922	1930	1939	rBV2	873400	1394185	12.68%	3.033%
13	16.153	2174	2181	2192	rBV	3269262	5157811	46.92%	11.220%
14	16.294	2199	2205	2211	rBV	636965	824238	7.50%	1.793%
15	17.410	2388	2395	2404	rBV2	1296931	2016722	18.35%	4.387%
16	18.362	2551	2557	2570	rBV	915217	1220591	11.10%	2.655%
17	20.007	2830	2837	2854	rBV	7635044	10992638	100.00%	23.912%
18	21.405	3070	3075	3088	rBV	886664	1194505	10.87%	2.598%
19	21.652	3110	3117	3127	rVB	1433539	2256185	20.52%	4.908%
20	23.092	3355	3362	3379	rBV	423125	903116	8.22%	1.965%
21	24.854	3651	3662	3675	rVB2	806812	2273122	20.68%	4.945%
22	25.571	3775	3784	3802	rBV2	153718	528982	4.81%	1.151%

Sum of corrected areas: 45971515

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022817\
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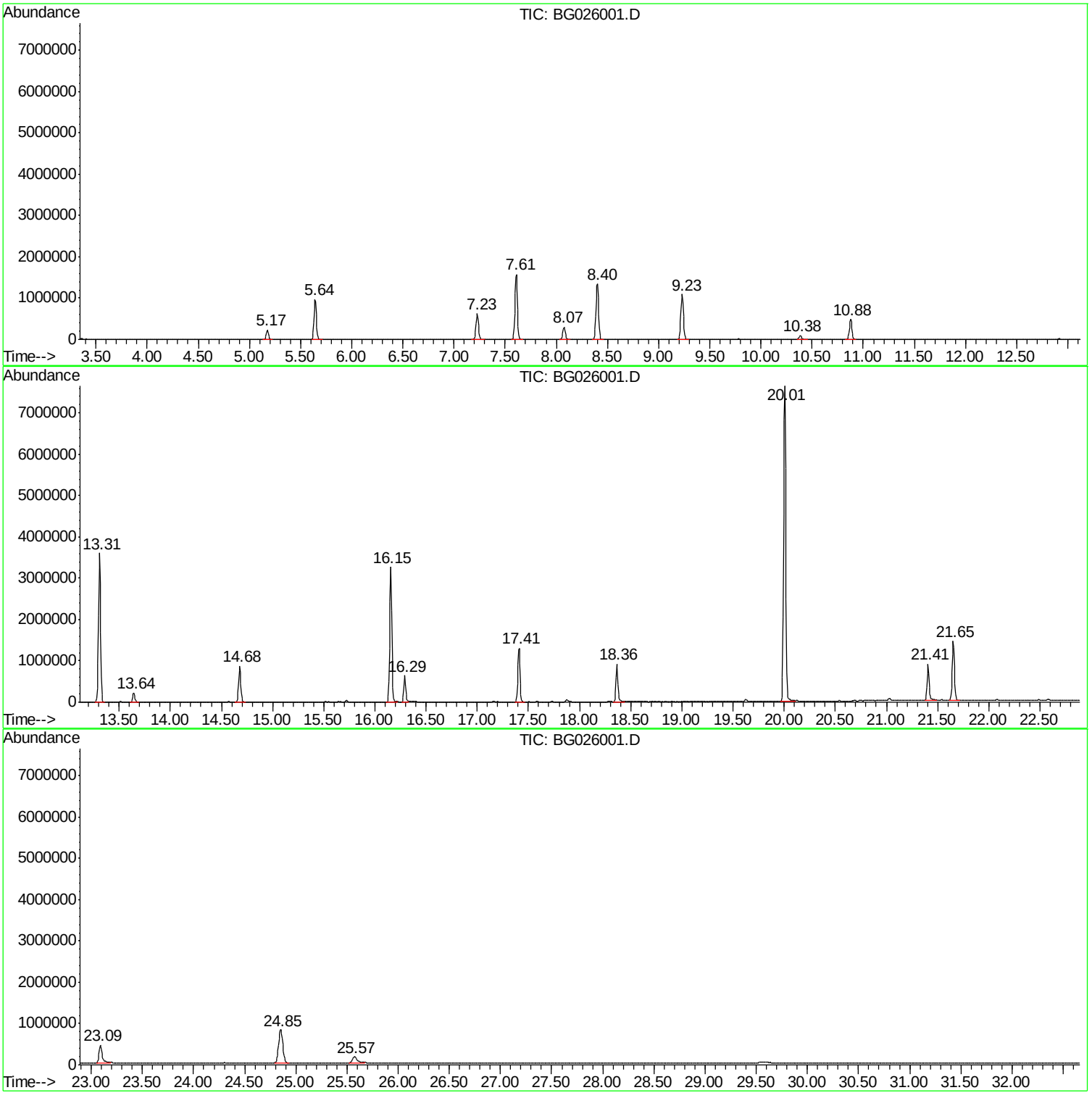
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FB-1-20170227

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.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

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022817\
Data File : BG026001.D
Acq On : 28 Feb 2017 17:39
Operator : SJ/MA
Sample : I2017-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-1-20170227

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.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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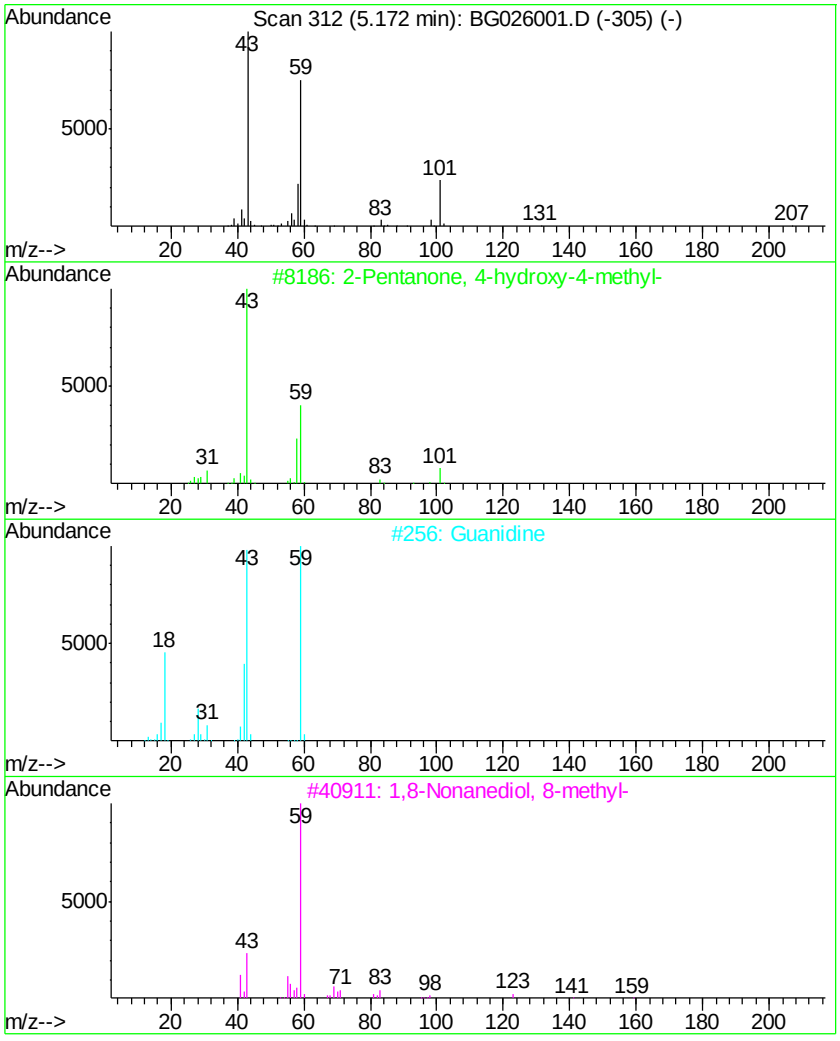
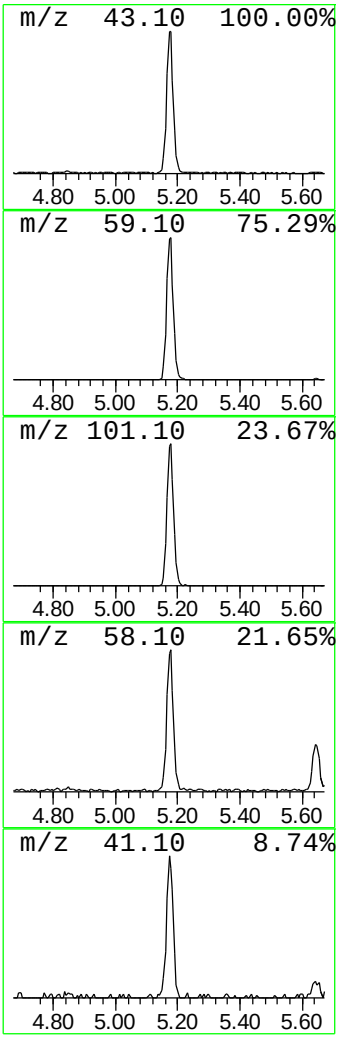
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	13.92 ng	356568	1,4-Dichlorobenzene-d4	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Guanidine	59	CH5N3	000113-00-8	47
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28
4	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	25
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022817\
Data File : BG026001.D
Acq On : 28 Feb 2017 17:39
Operator : SJ/MA
Sample : I2017-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-1-20170227

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.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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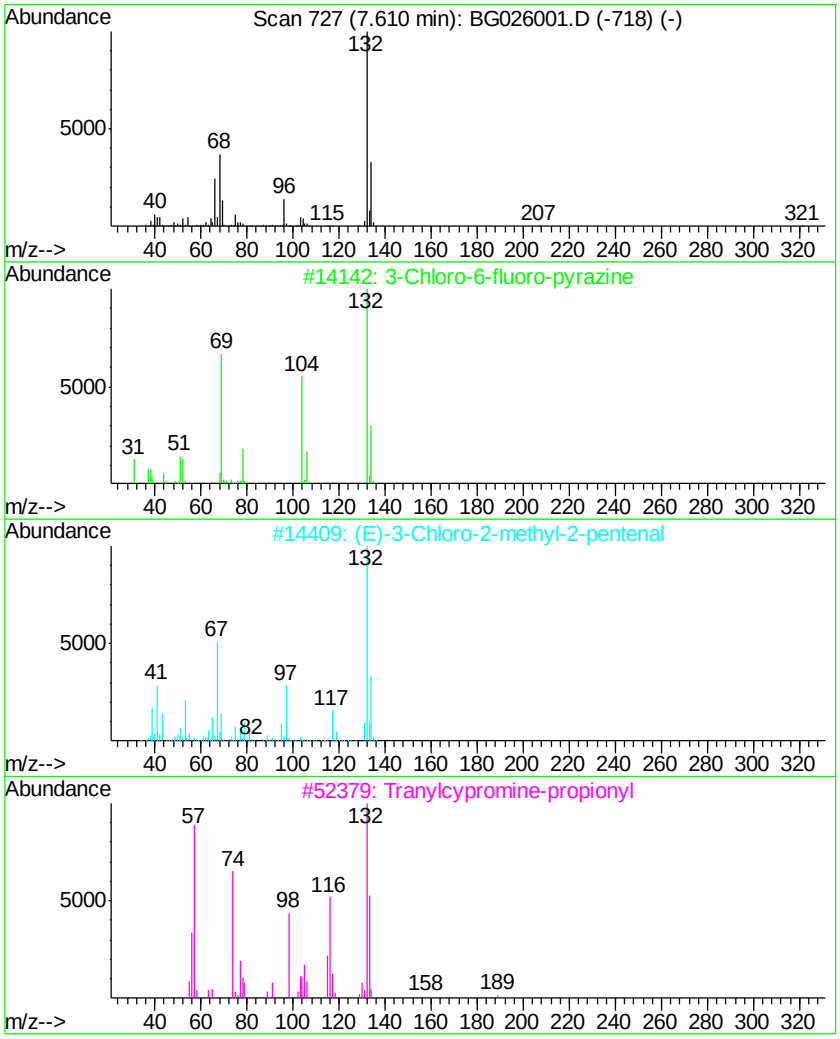
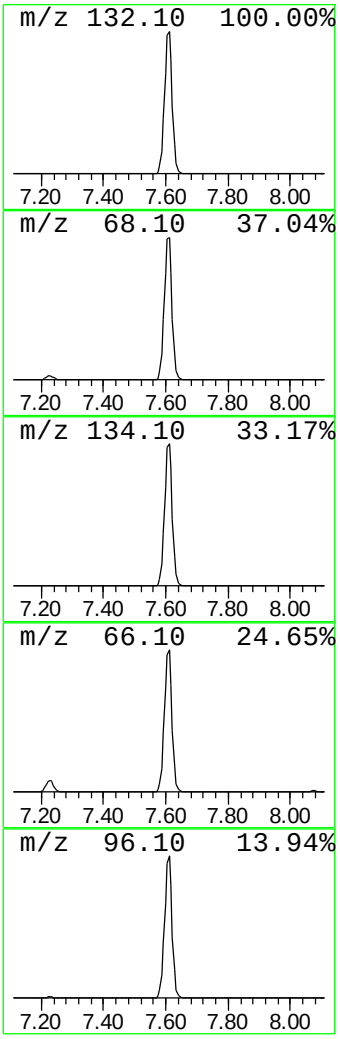
Peak Number 2 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	105.51 ng	2701810	1,4-Dichlorobenzene-d4	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022817\
Data File : BG026001.D
Acq On : 28 Feb 2017 17:39
Operator : SJ/MA
Sample : I2017-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-1-20170227

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.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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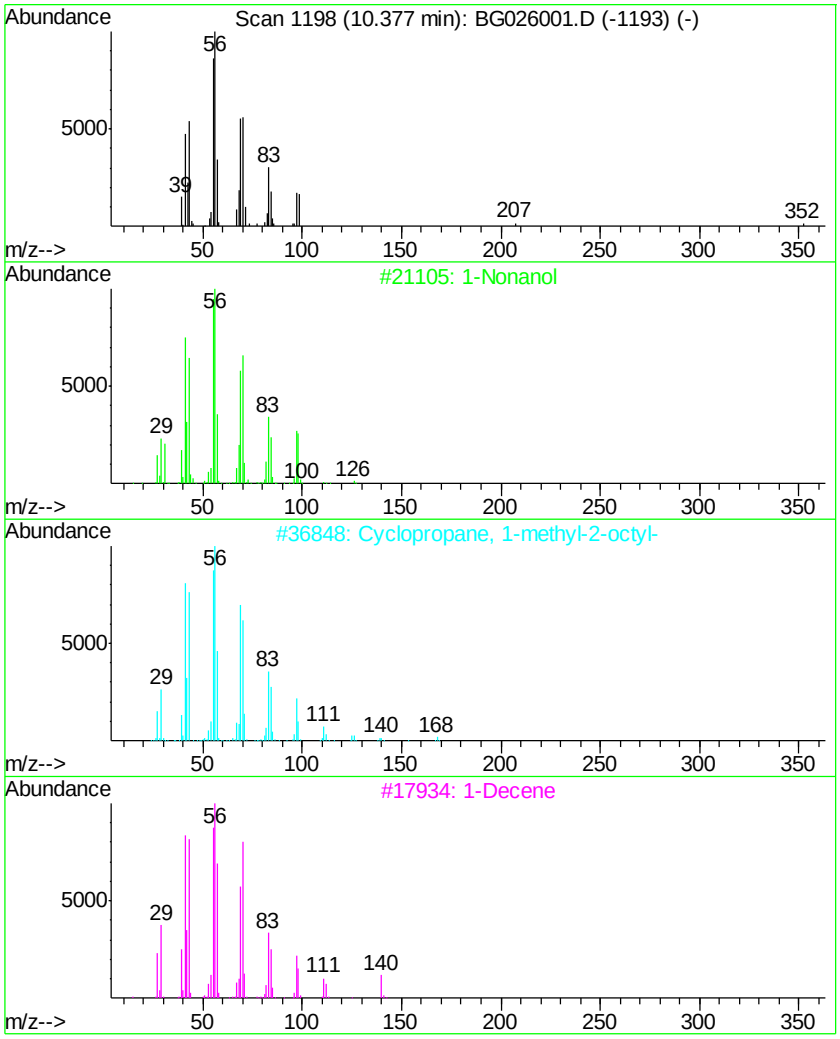
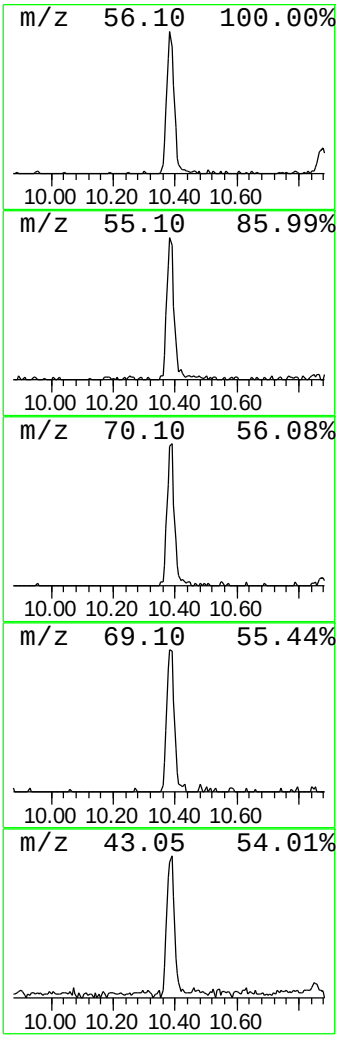
Peak Number 4 1-Nonanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	3.66 ng	153117	Naphthalene-d8	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	86
3	1-Decene	140	C10H20	000872-05-9	86
4	1-Octanol	130	C8H18O	000111-87-5	72
5	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	68





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022817\
Data File : BG026001.D
Acq On : 28 Feb 2017 17:39
Operator : SJ/MA
Sample : I2017-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-1-20170227

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.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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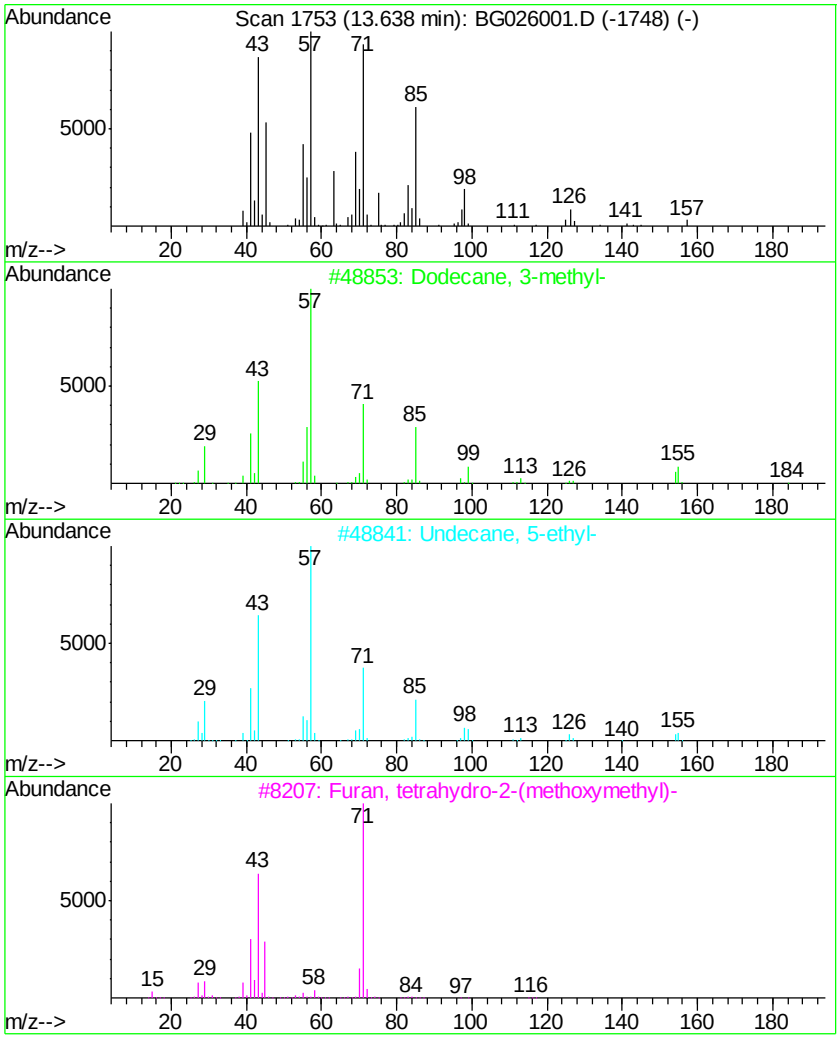
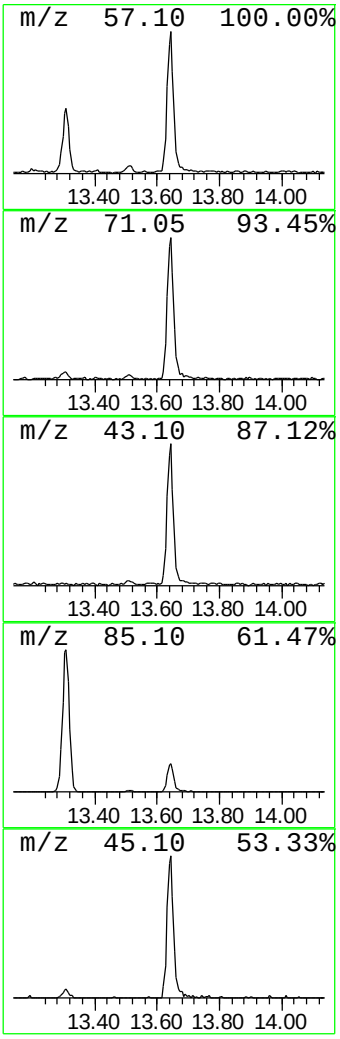
Peak Number 5 unknown13.64 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	4.68 ng	326268	Acenaphthene-d10	14.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 3-methyl-	184	C13H28	017312-57-1	47
2	Undecane, 5-ethyl-	184	C13H28	017453-94-0	47
3	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	43
4	Propanoic acid, 2-chloro-, 1-met...	178	C8H15ClO2	088736-64-5	38
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	35





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022817\
Data File : BG026001.D
Acq On : 28 Feb 2017 17:39
Operator : SJ/MA
Sample : I2017-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-1-20170227

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

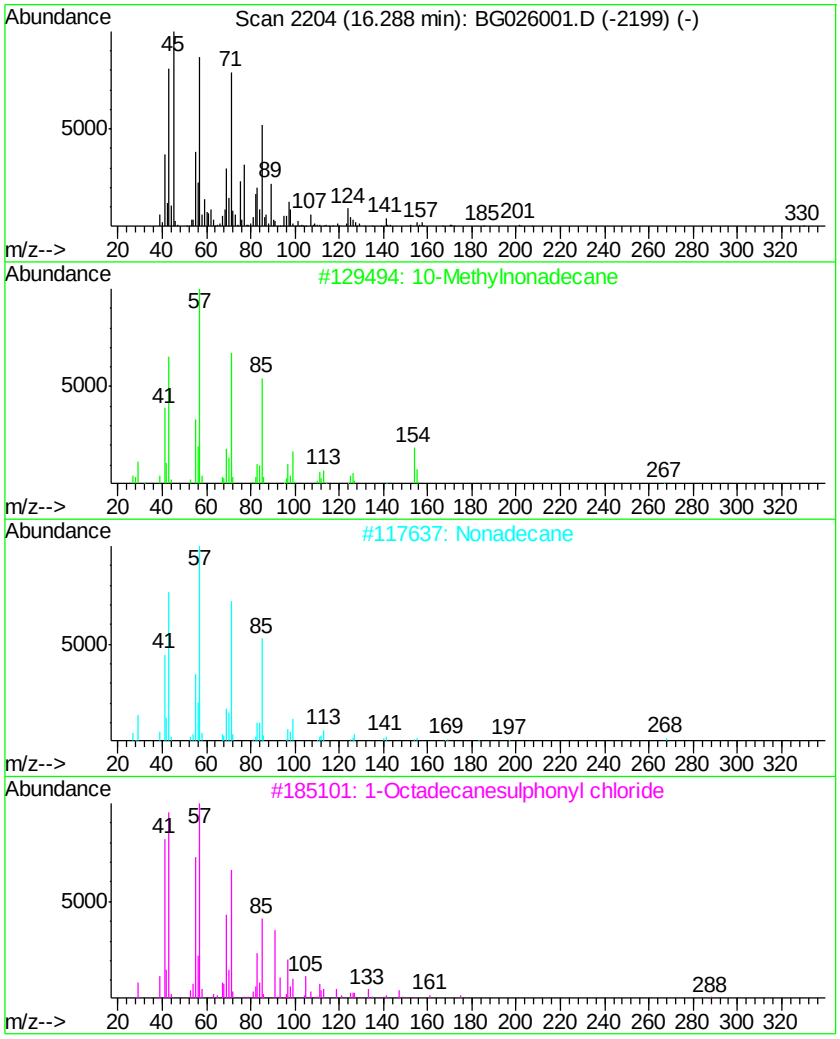
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

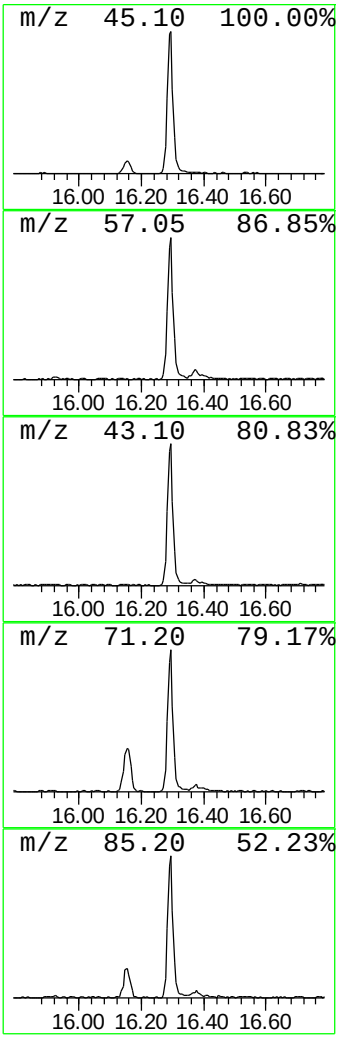
****

Peak Number 6 unknown16.29 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	8.17 ng	824238	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	38
2	Nonadecane	268	C19H40	000629-92-5	38
3	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	35
4	Diethylene glycol hexyl ether	190	C10H22O3	000112-59-4	35
5	Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	27





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022817\
Data File : BG026001.D
Acq On : 28 Feb 2017 17:39
Operator : SJ/MA
Sample : I2017-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-1-20170227

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.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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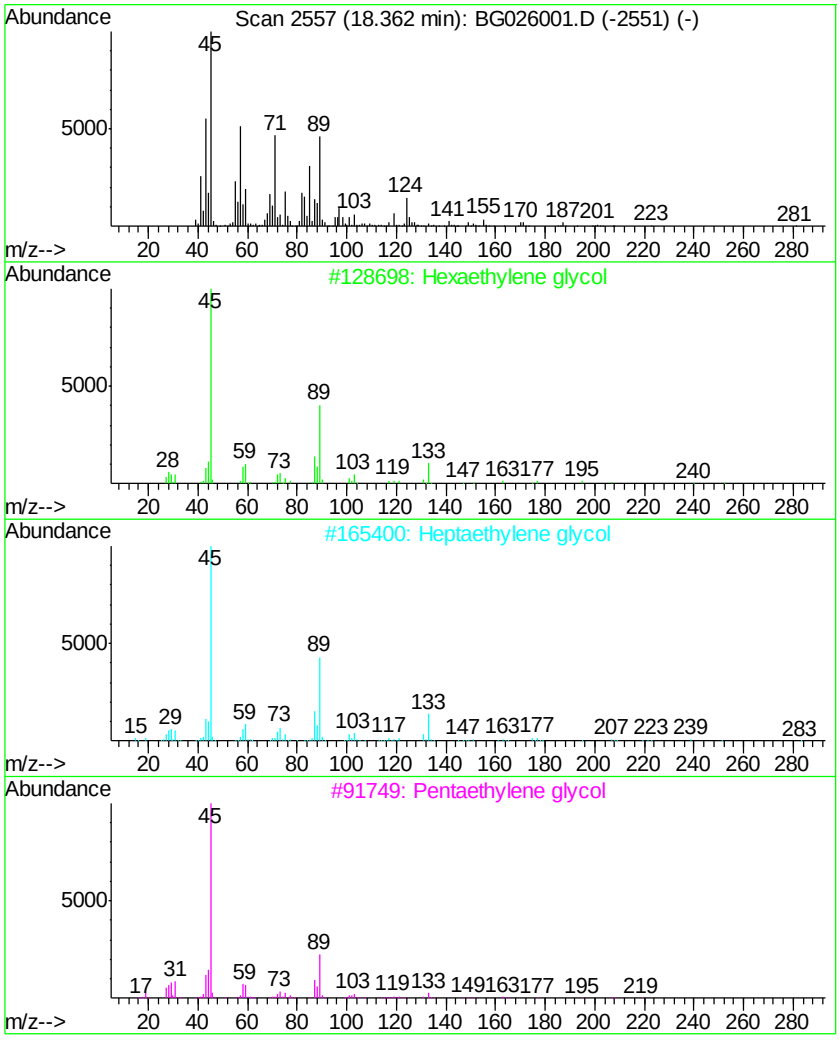
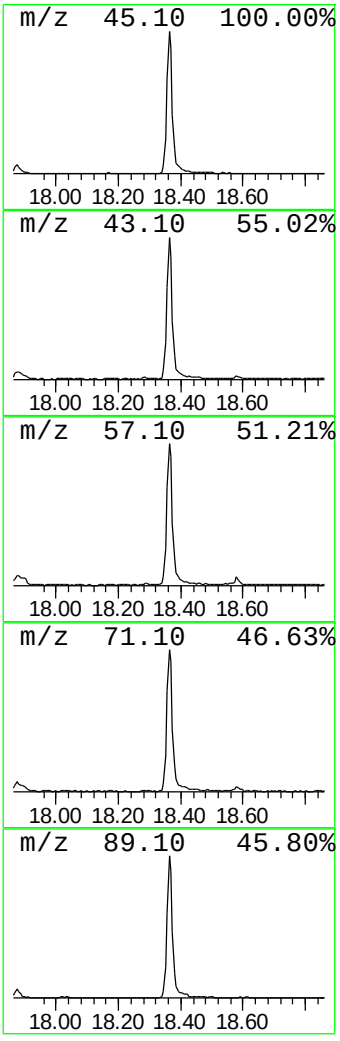
Peak Number 7 Hexaethylene glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	12.10 ng	1220590	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	50
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	49
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	47
4	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	47
5	Methoxyacetic acid, 3-tridecyl e...	272	C16H32O3	1000282-04-6	47





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Sample : I2017-16
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-1-20170227

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.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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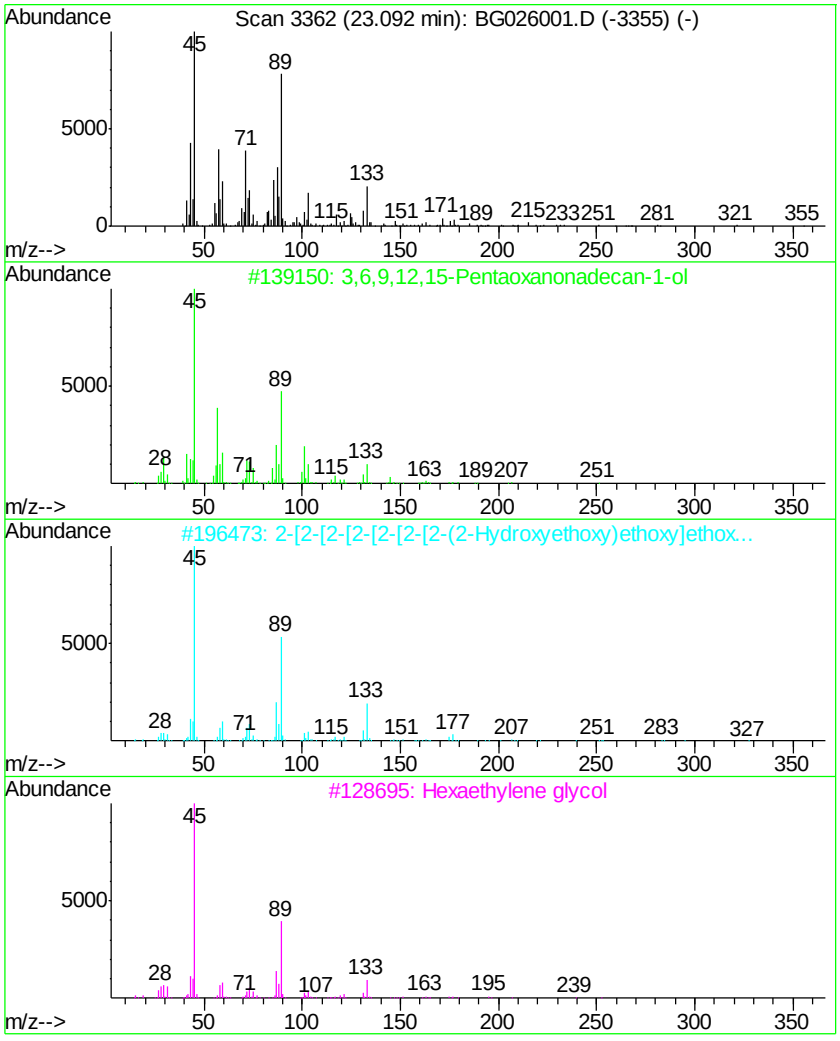
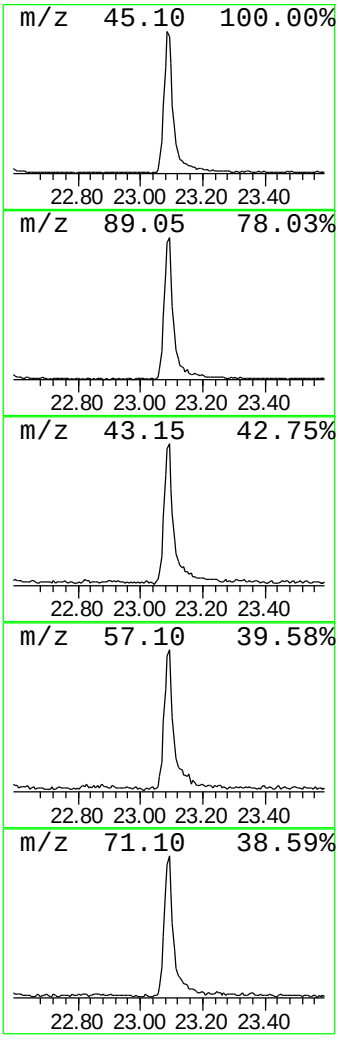
Peak Number 9 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	8.01 ng	903116	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	86
2	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	83
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	83
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	80
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	80





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022817\
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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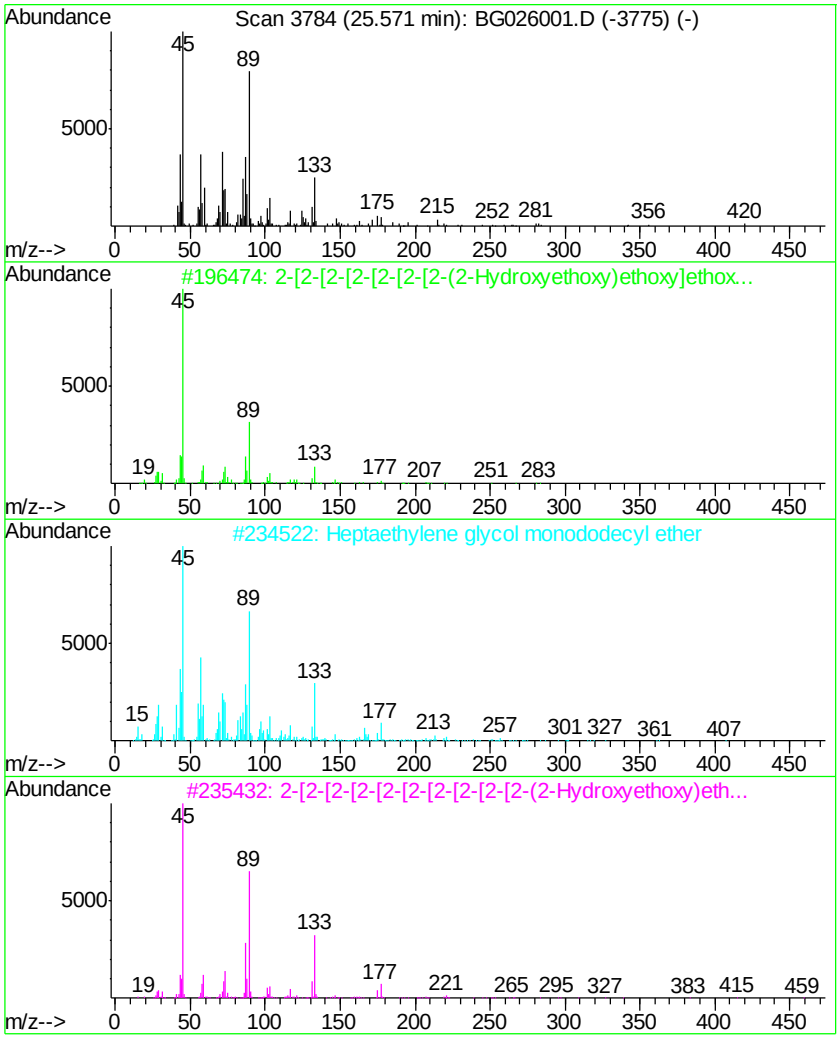
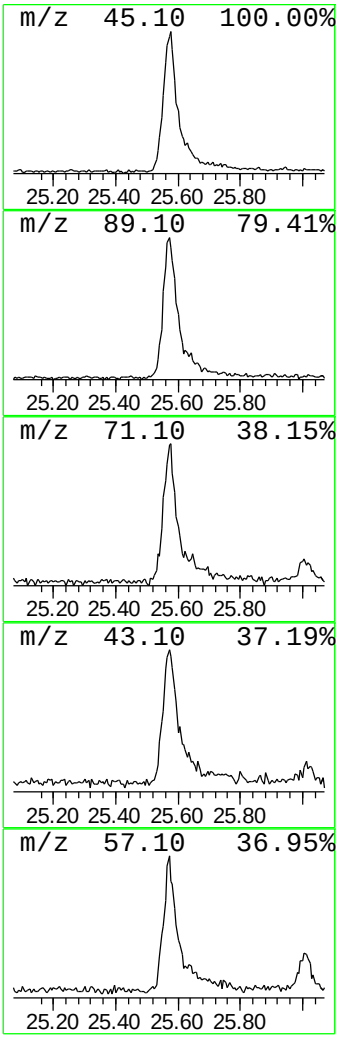
Peak Number 10 2-[2-[2-[2-[2-[2-[2-(2-Hydr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.57	4.65 ng	528982	Perylene-d12	24.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	83
2	Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	83
3	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	80
4	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	72
5	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022817\
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Operator : SJ/MA
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG021717.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
2-Pentanone, 4-hy...	5.17	13.9	ng	356568	1	8.08	512166	20.0
unknown7.61	7.61	105.5	ng	2701810	1	8.08	512166	20.0
1-Nonanol	10.38	3.7	ng	153117	2	10.88	835930	20.0
unknown13.64	13.64	4.7	ng	326268	3	14.68	1394190	20.0
unknown16.29	16.29	8.2	ng	824238	4	17.40	2016720	20.0
Hexaethylene glycol	18.36	12.1	ng	1220590	4	17.40	2016720	20.0
3,6,9,12,15-Penta...	23.09	8.0	ng	903116	5	21.65	2256190	20.0
2-[2-[2-[2-[2-[2-...	25.57	4.7	ng	528982	6	24.85	2273120	20.0