LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
Data File : BG051179.D
Acq On : 22 Nov 2021 20:58
Operator : CG/JU
Sample : M4786-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-357

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-BG111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051179.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.947	52	78	82	rBV	1651414	8673977	100.00%	20.643%
2	5.040	255	264	273	rBV	71416	130179	1.50%	0.310%
3	5.751	378	385	400	rVB	508286	860879	9.92%	2.049%
4	7.366	650	660	671	rVB	538444	969758	11.18%	2.308%
5	8.201	796	802	817	rVB	114431	197714	2.28%	0.471%
6	9.382	995	1003	1014	rVB	319468	581395	6.70%	1.384%
7	11.033	1275	1284	1291	rBV	169701	304393	3.51%	0.724%
8	13.453	1688	1696	1707	rVB	862934	1334864	15.39%	3.177%
9	13.818	1742	1758	1773	rBV	427769	1472681	16.98%	3.505%
10	14.734	1908	1914	1925	rBV	254320	391778	4.52%	0.932%
11	14.834	1925	1931	1939	rVB	275040	447656	5.16%	1.065%
12	16.326	2178	2185	2206	rBV	441009	842619	9.71%	2.005%
13	17.219	2330	2337	2348	rBV	837755	1249176	14.40%	2.973%
14	17.584	2393	2399	2404	rBV	345780	525237	6.06%	1.250%
15	19.211	2668	2676	2696	rBV	1733680	2693249	31.05%	6.410%
16	20.175	2834	2840	2846	rVB	1417906	1849024	21.32%	4.400%
17	20.774	2934	2942	2962	rBV	2766279	4699004	54.17%	11.183%
18	21.473	3056	3061	3070	rVB4	65870	132993	1.53%	0.317%
19	21.726	3099	3104	3112	rVB	243173	356365	4.11%	0.848%
20	21.885	3124	3131	3137	rBV	303670	559191	6.45%	1.331%
21	22.349	3198	3210	3231	rBV	2350946	5776239	66.59%	13.747%
22	24.505	3561	3577	3596	rBV	1405254	4896107	56.45%	11.652%
23	25.292	3702	3711	3721	rVB2	164553	499155	5.75%	1.188%
24	27.866	4130	4149	4173	rBV	517143	2575253	29.69%	6.129%

Sum of corrected areas: 42018886

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ClientSampleId :
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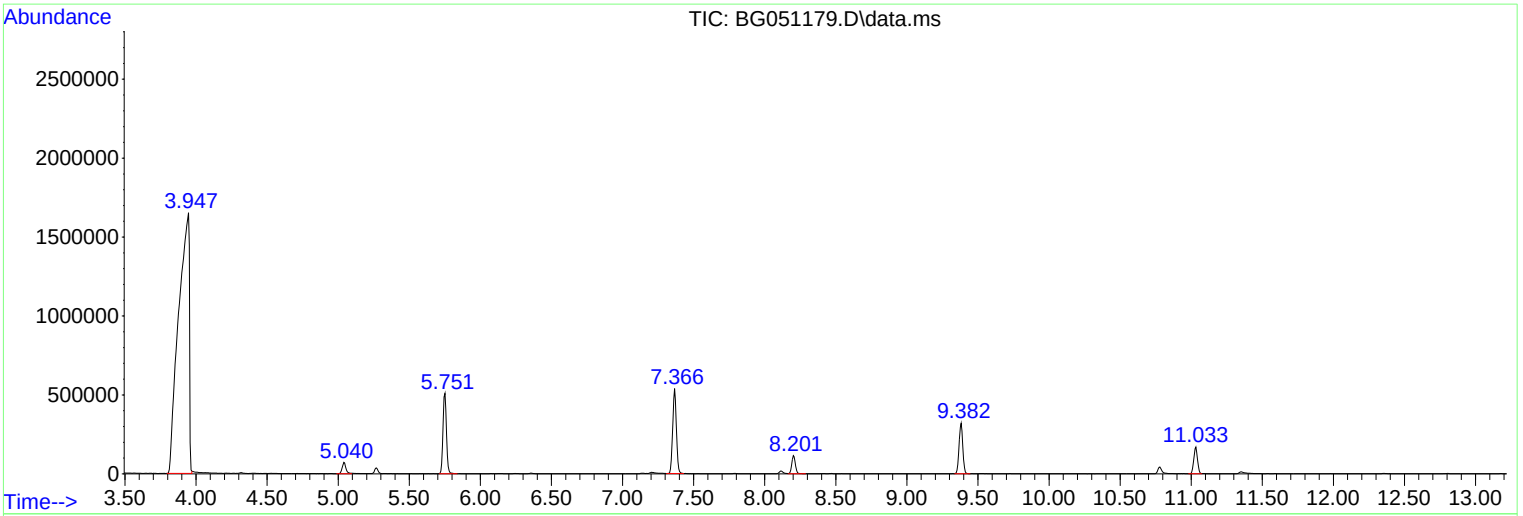
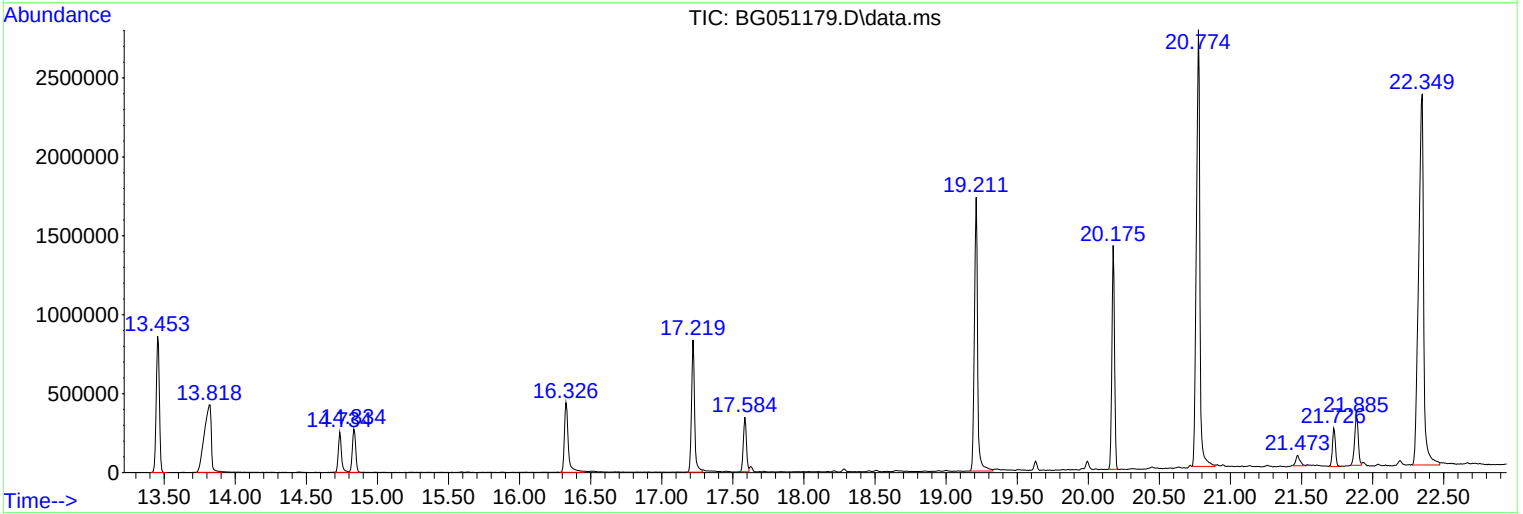
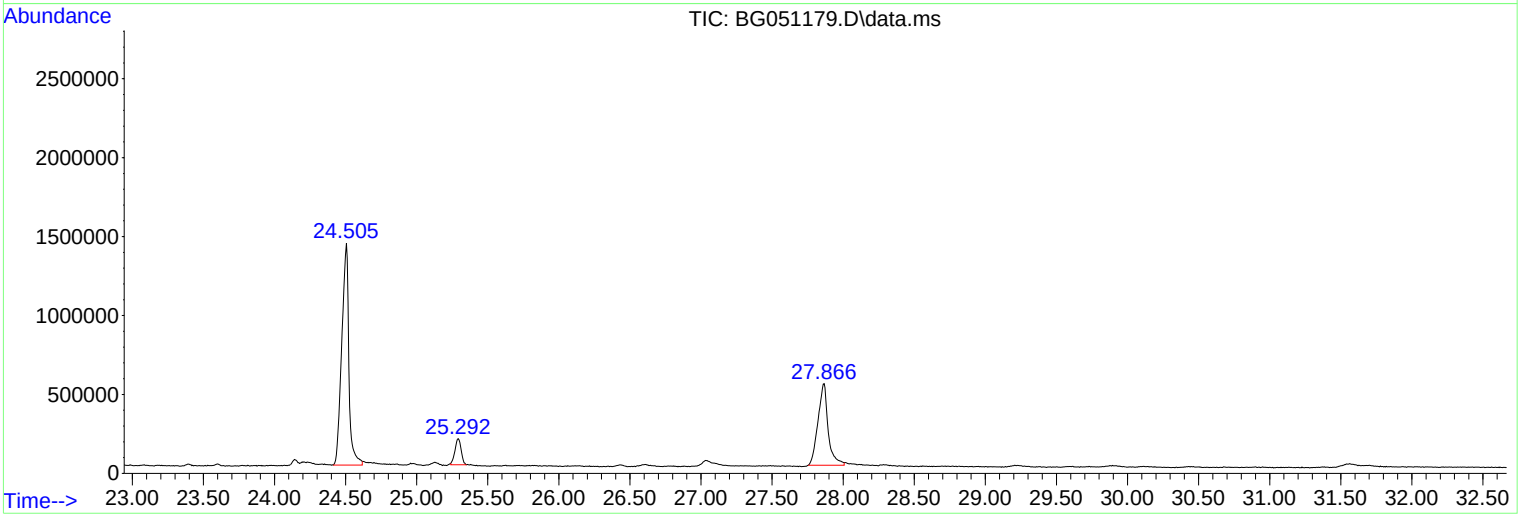
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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TIC Library : C:\Database\NIST20.L
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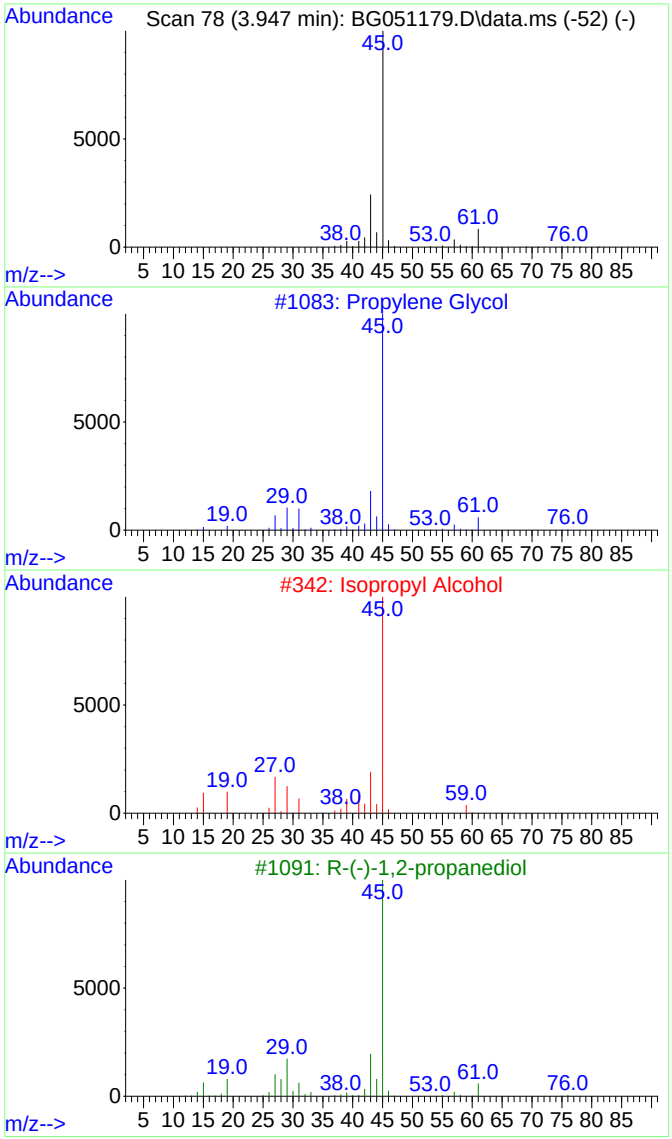
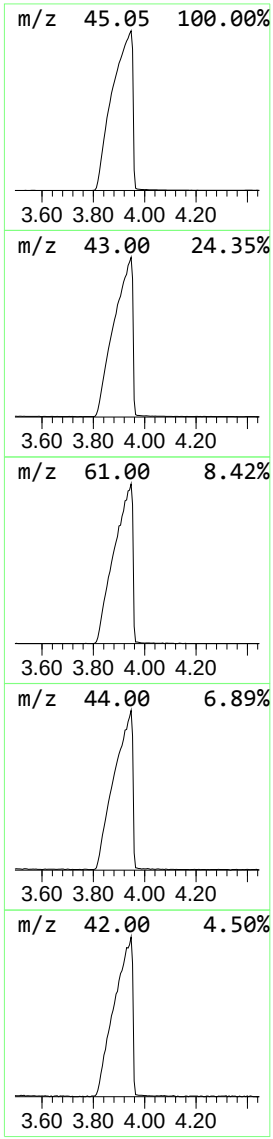
Peak Number 1 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.947	877.43 ng	8673980	1,4-Dichlorobenzene-d4	8.201

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4	3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	40
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40





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Sample : M4786-03
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
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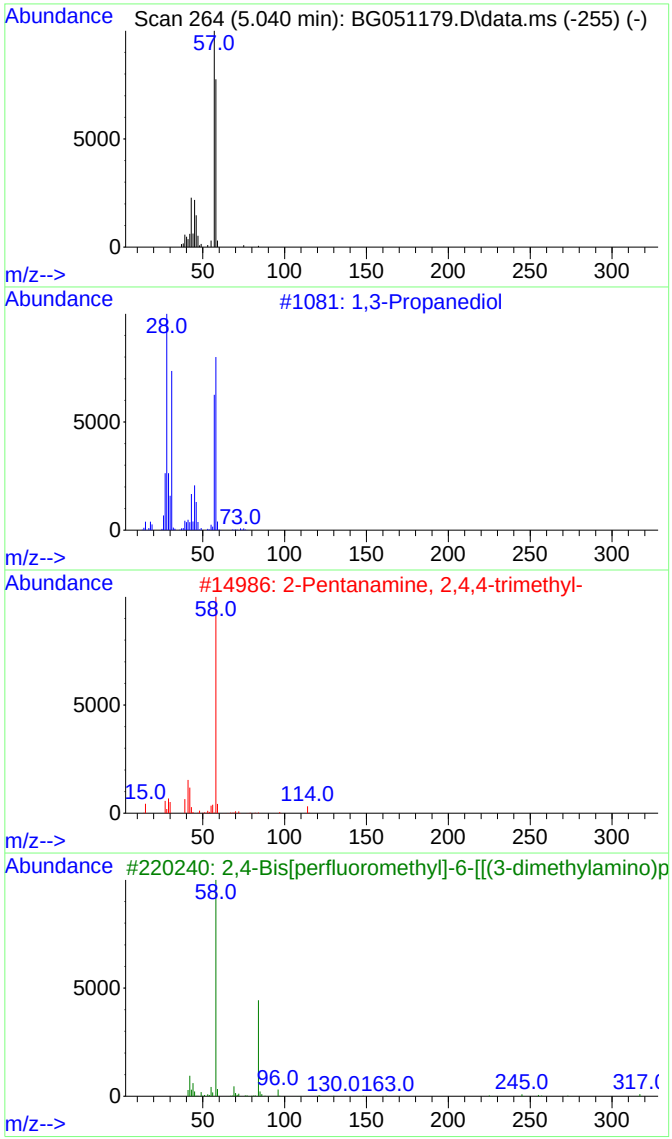
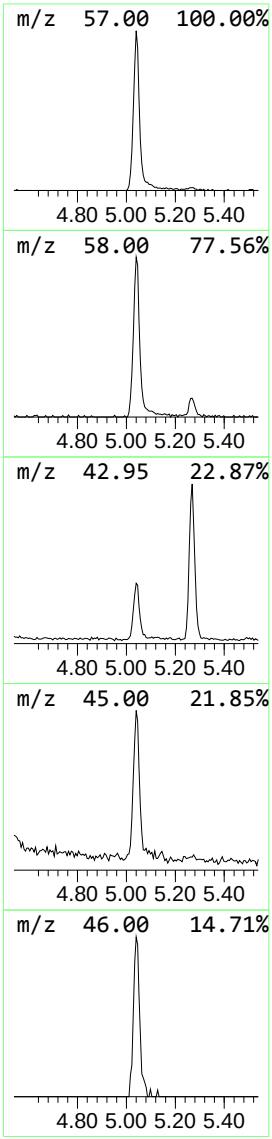
Peak Number 2 1,3-Propanediol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	13.17 ng	130179	1,4-Dichlorobenzene-d4	8.201

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Propanediol	76	C3H8O2	000504-63-2	78
2	2-Pentanamine, 2,4,4-trimethyl-	129	C8H19N	000107-45-9	38
3	2,4-Bis[perfluoromethyl]-6-[[(3-...	317	C10H13F6N5	1000253-62-7	28
4	Propanal	58	C3H6O	000123-38-6	9
5	Diborane(6), .mu.-mercapto-	60	B2H6S	022548-43-2	9





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Sample : M4786-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
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TIC Library : C:\Database\NIST20.L
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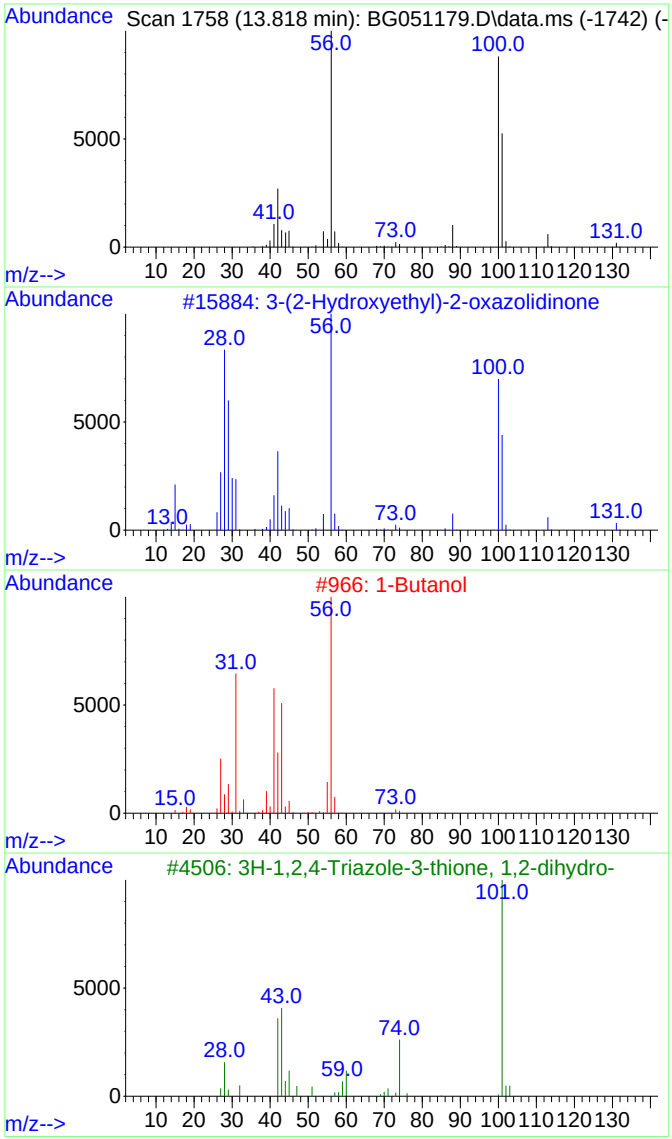
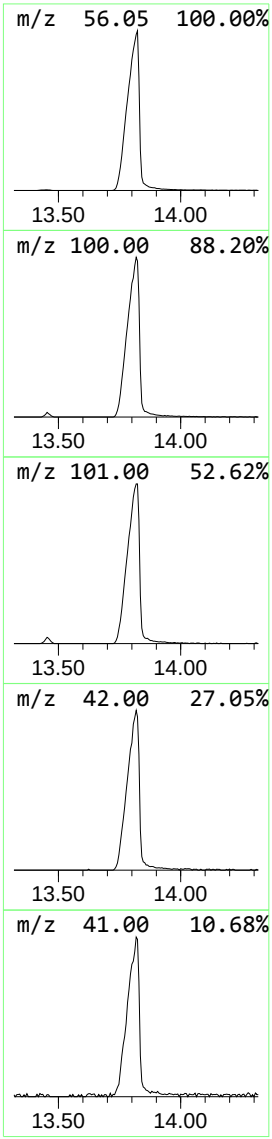
Peak Number 3 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.818	65.80 ng	1472680	Acenaphthene-d10	14.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	91
2	1-Butanol	74	C4H10O	000071-36-3	27
3	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	10
4	Imidazole, 5-fluoro-4-methyl-	100	C4H5FN2	041367-01-5	9
5	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9





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TIC Library : C:\Database\NIST20.L
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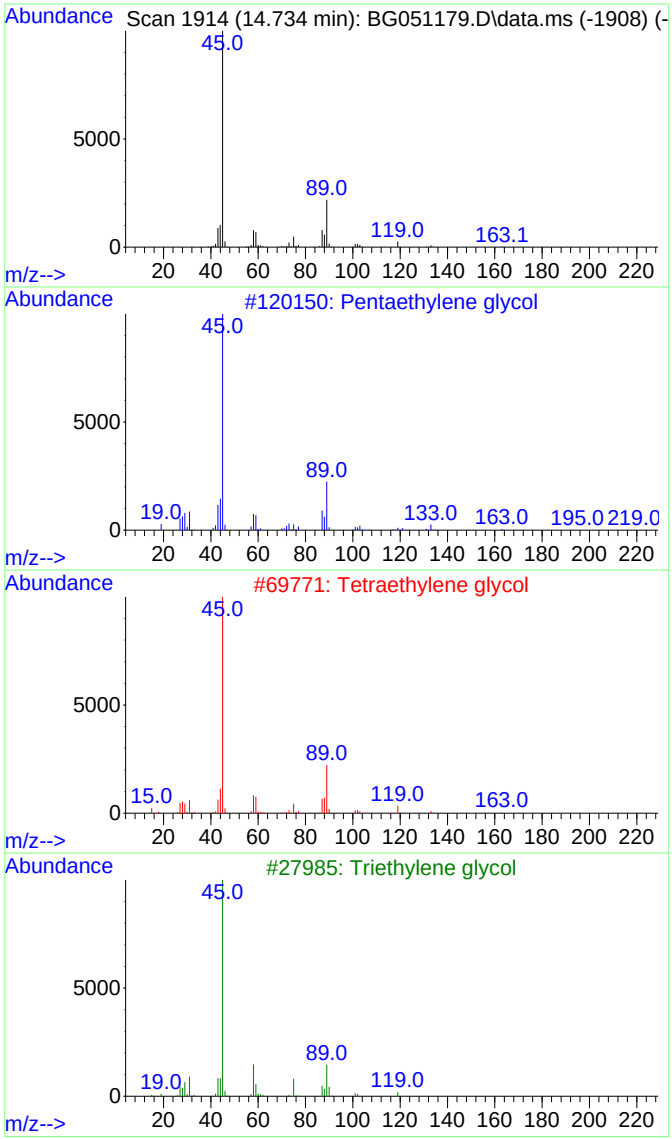
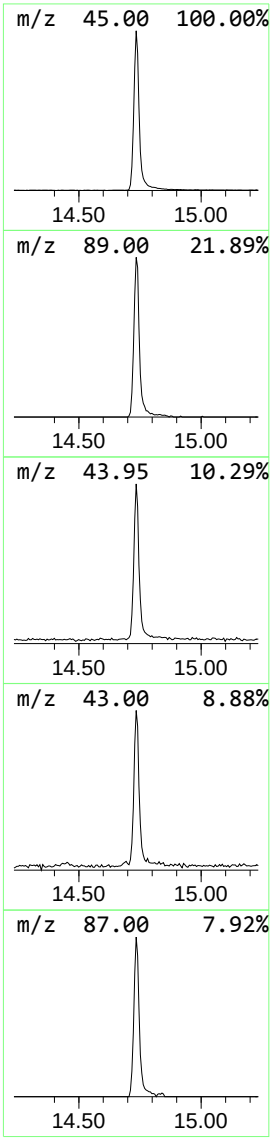
Peak Number 4 Pentaethylene glycol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.734	17.50 ng	391778	Acenaphthene-d10	14.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	90
2	Tetraethylene glycol	194	C8H18O5	000112-60-7	90
3	Triethylene glycol	150	C6H14O4	000112-27-6	83
4	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	83
5	Hexaethylene glycol	282	C12H26O7	002615-15-8	83





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Sample : M4786-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
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TIC Library : C:\Database\NIST20.L
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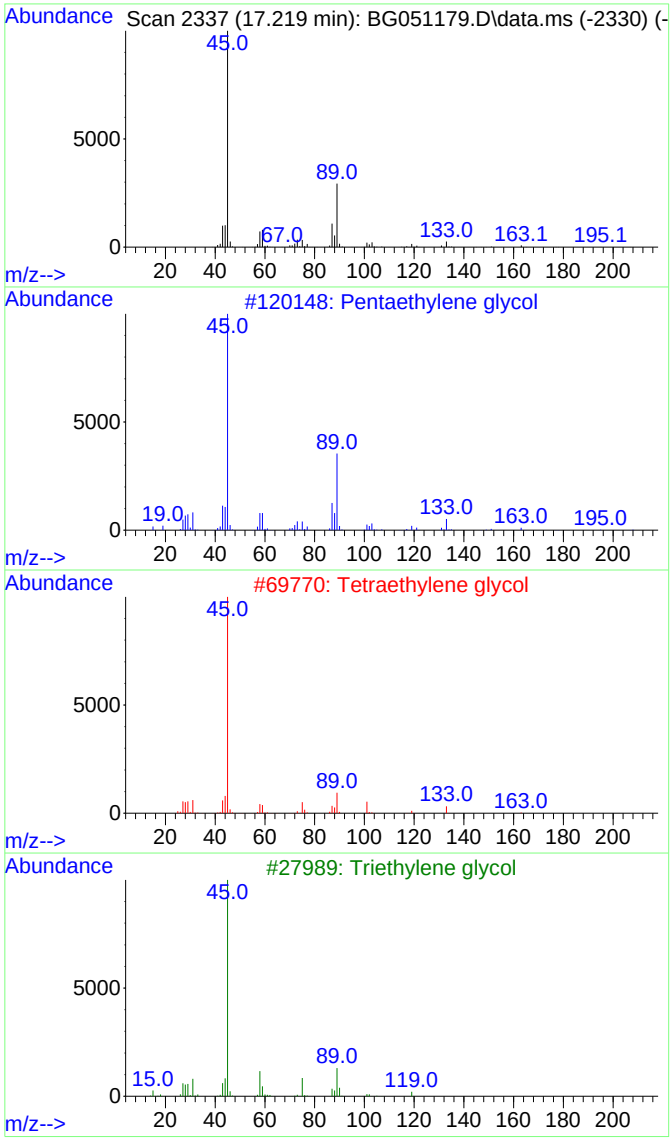
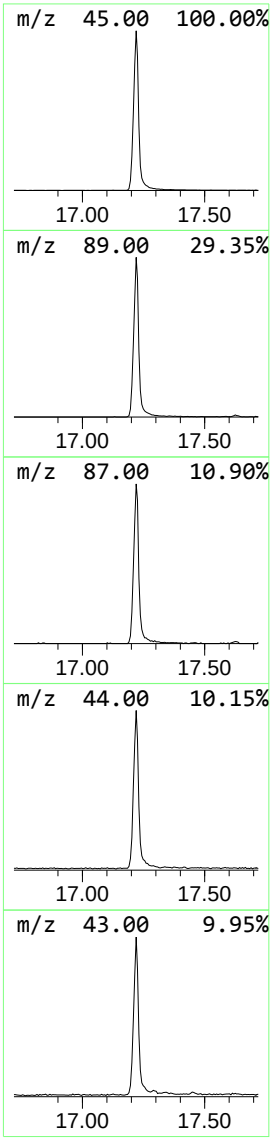
Peak Number 5 Tetraethylene glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.220	47.57 ng	1249180	Phenanthrene-d10	17.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	90
2	Tetraethylene glycol	194	C8H18O5	000112-60-7	78
3	Triethylene glycol	150	C6H14O4	000112-27-6	78
4	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	64
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	64





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TIC Library : C:\Database\NIST20.L
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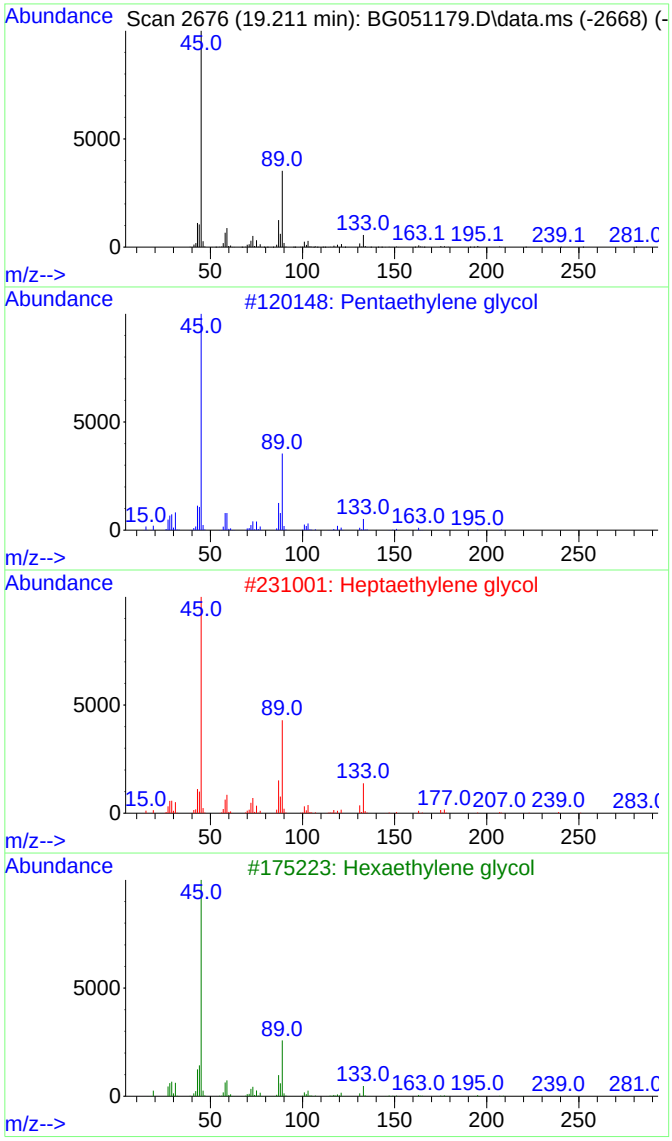
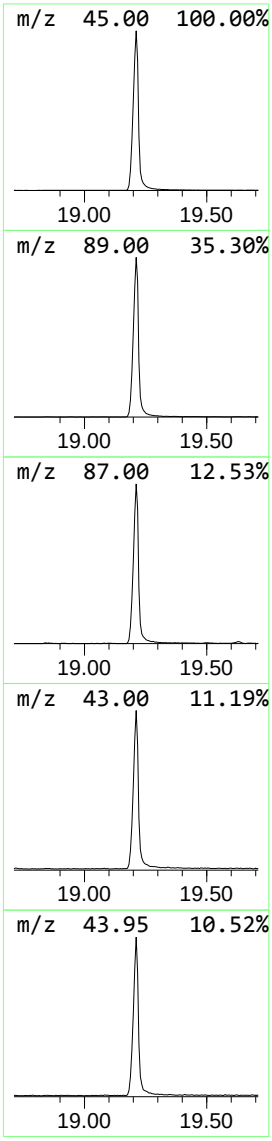
Peak Number 6 Heptaethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.211	102.55 ng	2693250	Phenanthrene-d10	17.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	91
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	90
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	86
4	Tetraethyleneglycol monomethylether	208	C9H20O5	023783-42-8	83
5	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	83





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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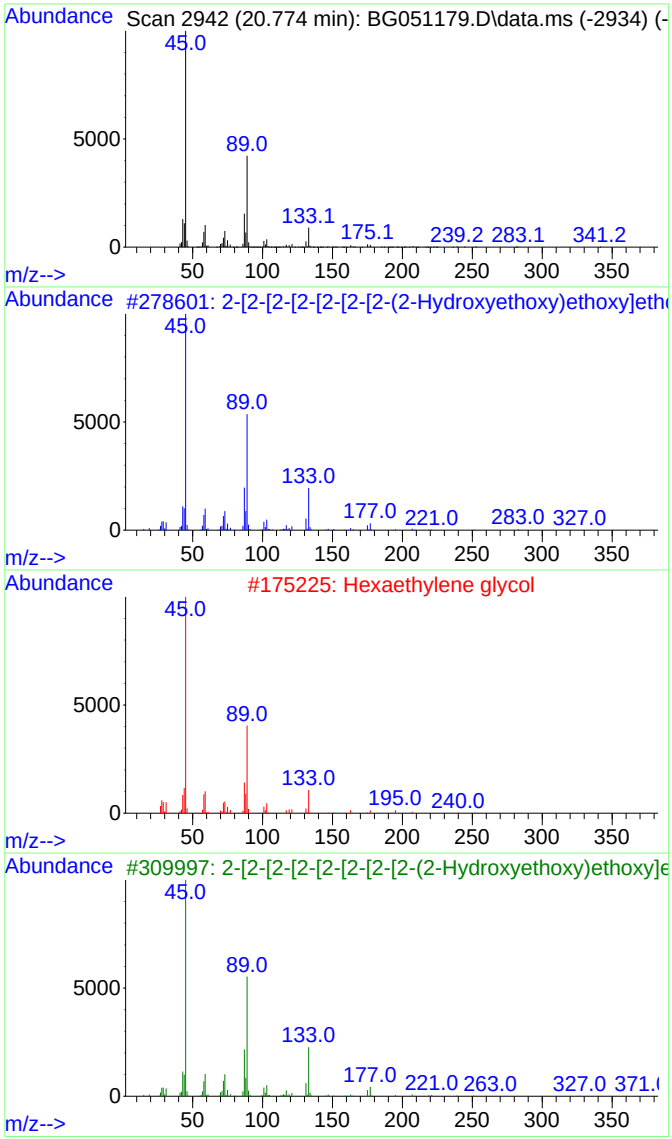
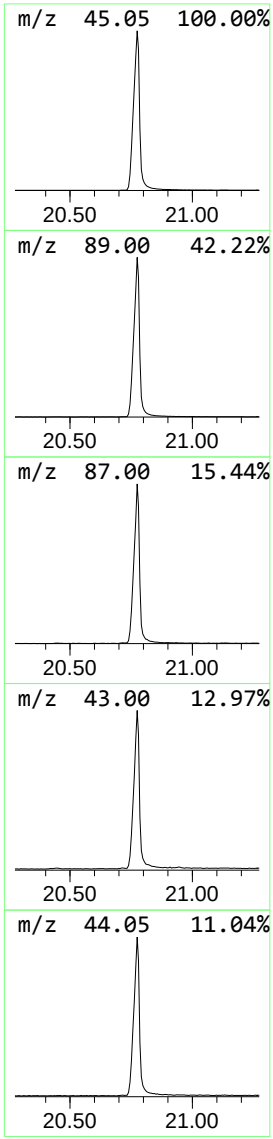
Peak Number 7 unknown20.774 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.774	168.06 ng	4699000	Chrysene-d12	21.885

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	91
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	91
4	Pentaethylene glycol	238	C10H22O6	004792-15-8	83
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	83





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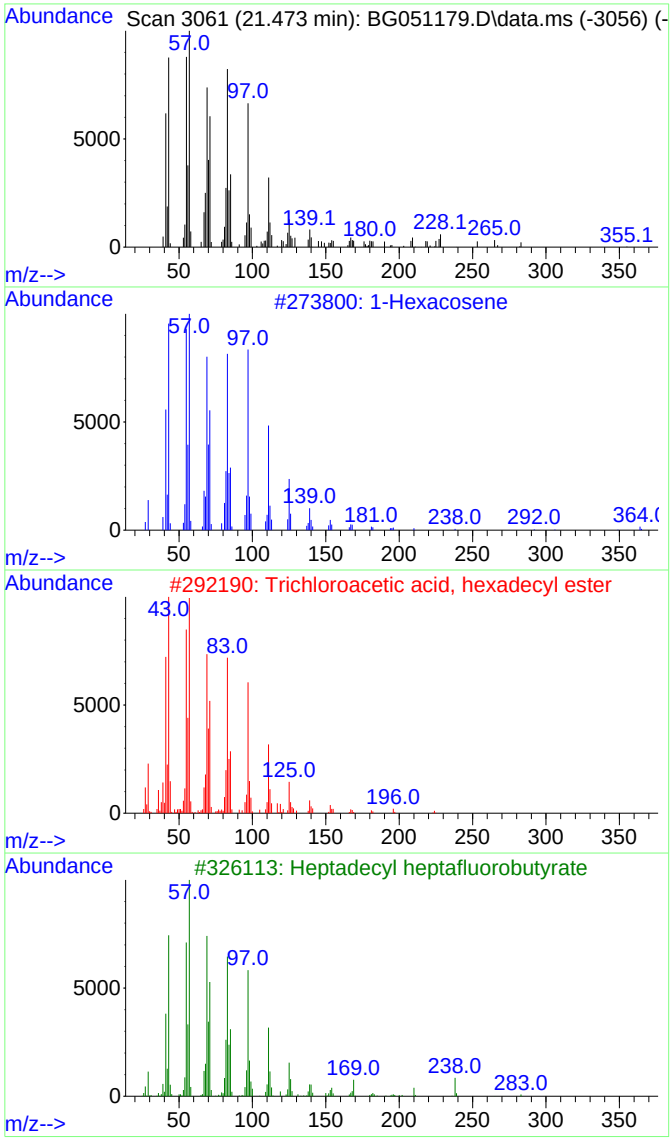
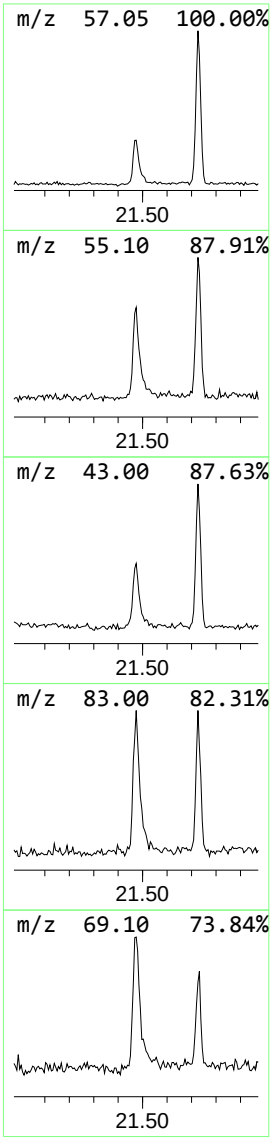
Peak Number 8 1-Hexacosene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.473	4.76 ng	132993	Chrysene-d12	21.885

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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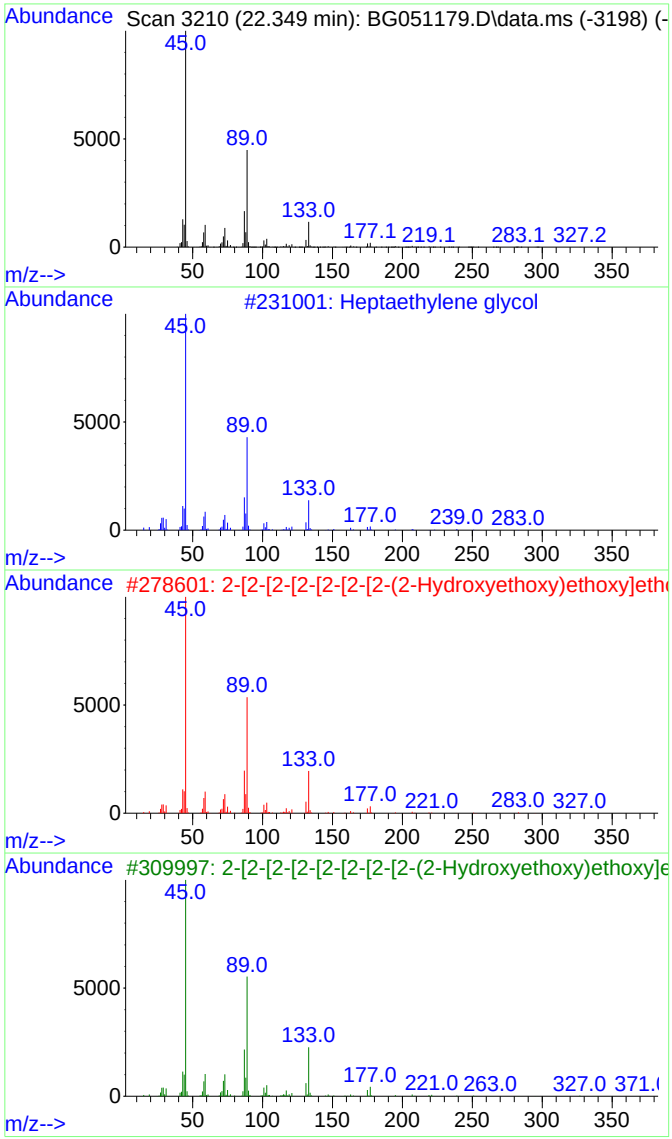
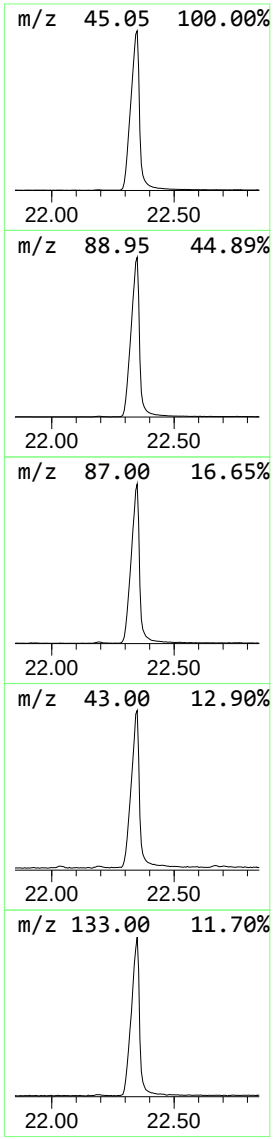
Peak Number 9 unknown22.349 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.349	206.59 ng	5776240	Chrysene-d12	21.885

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	91
2	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	91
4	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	006809-70-7	90
5	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	005579-66-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
Data File : BG051179.D
Acq On : 22 Nov 2021 20:58
Operator : CG/JU
Sample : M4786-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-357

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

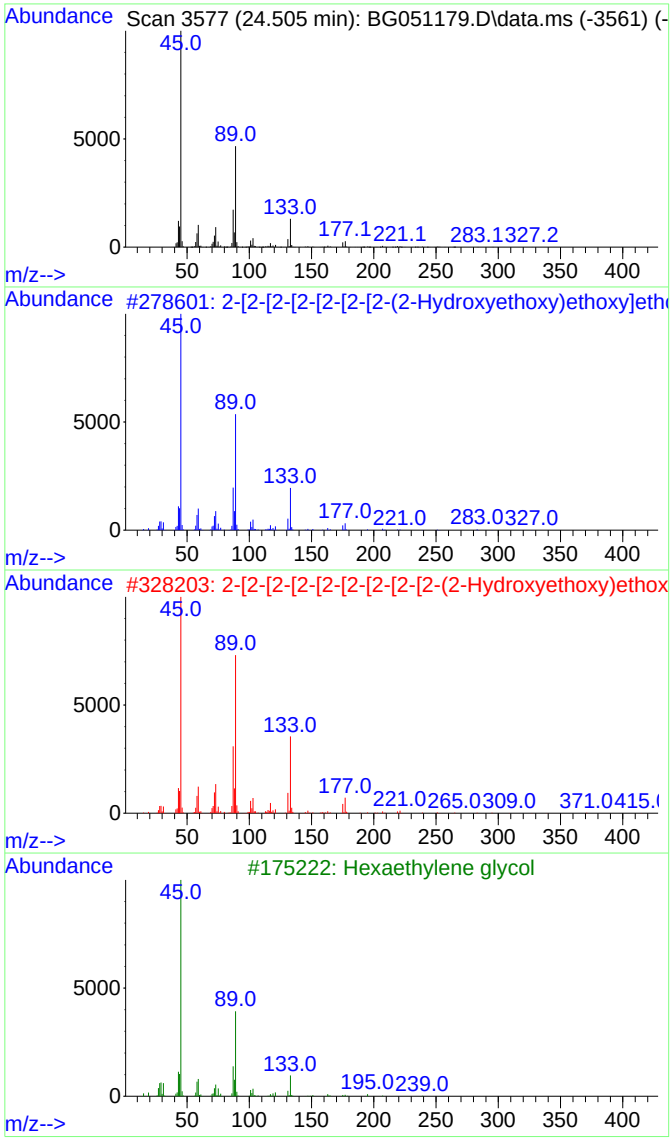
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

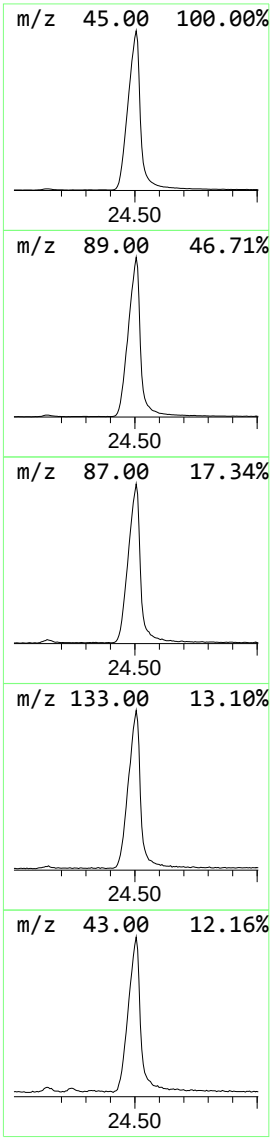
****

Peak Number 10 unknown24.505 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.505	196.18 ng	4896110	Perylene-d12	25.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
2	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	005579-66-8	91
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	91
4	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	90
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
Data File : BG051179.D
Acq On : 22 Nov 2021 20:58
Operator : CG/JU
Sample : M4786-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-357

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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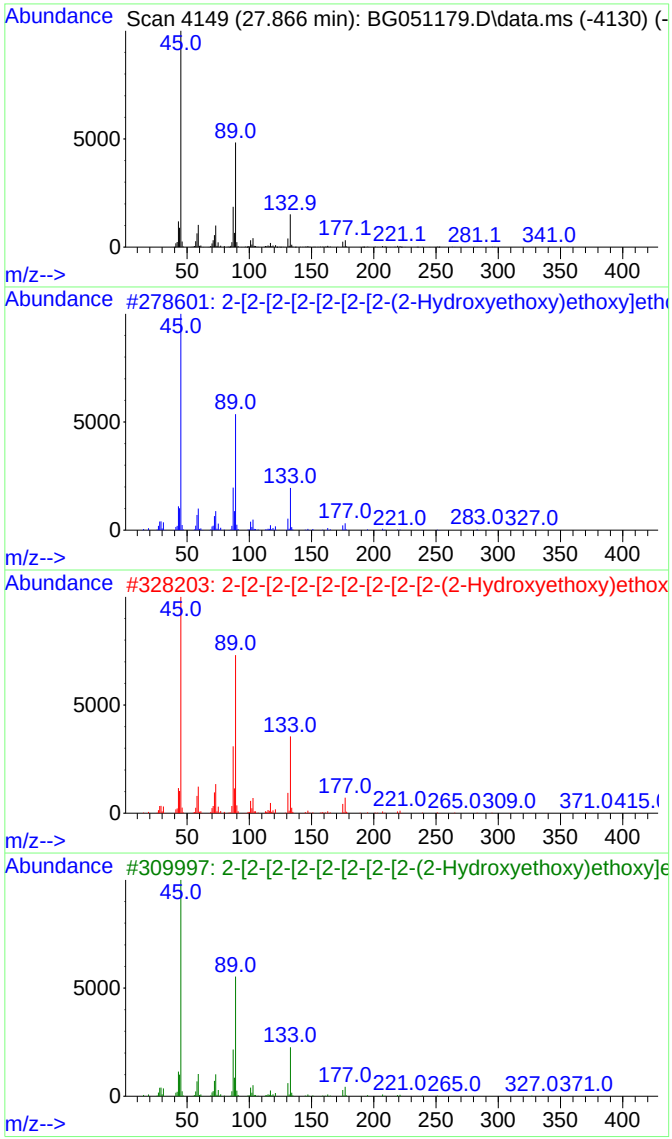
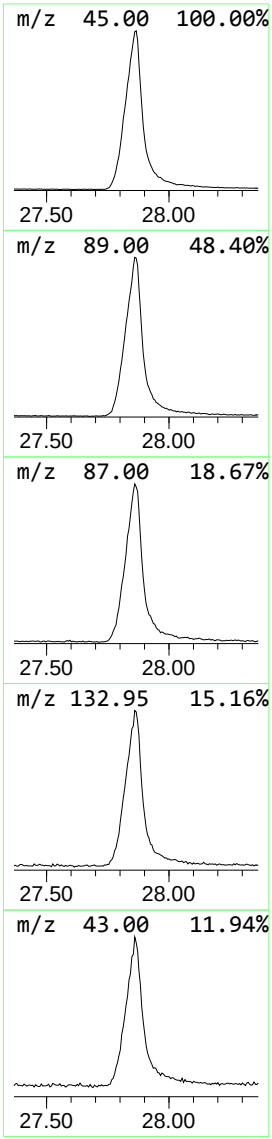
Peak Number 11 unknown27.866 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.866	103.19 ng	2575250	Perylene-d12	25.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
2	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	005579-66-8	91
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	91
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	91
5	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
Data File : BG051179.D
Acq On : 22 Nov 2021 20:58
Operator : CG/JU
Sample : M4786-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-357

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propylene Glycol	3.947	877.4	ng	8673980	1	8.201	197714	20.0
1,3-Propanediol	5.040	13.2	ng	130179	1	8.201	197714	20.0
3-(2-Hydroxyeth...	13.818	65.8	ng	1472680	3	14.834	447656	20.0
Pentaethylene g...	14.734	17.5	ng	391778	3	14.834	447656	20.0
Tetraethylene g...	17.220	47.6	ng	1249180	4	17.584	525237	20.0
Heptaethylene g...	19.211	102.6	ng	2693250	4	17.584	525237	20.0
unknown20.774	20.774	168.1	ng	4699000	5	21.885	559191	20.0
1-Hexacosene	21.473	4.8	ng	132993	5	21.885	559191	20.0
unknown22.349	22.349	206.6	ng	5776240	5	21.885	559191	20.0
unknown24.505	24.505	196.2	ng	4896110	6	25.292	499155	20.0
unknown27.866	27.866	103.2	ng	2575250	6	25.292	499155	20.0