

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030521\
 Data File : BG048350.D
 Acq On : 5 Mar 2021 23:09
 Operator : CG/JU
 Sample : M1553-08
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 1729

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-BG021021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048350.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.122	463	474	484	rBV	3182654	6032961	4.21%	1.556%
2	8.155	812	820	837	rBV	1519653	3225095	2.25%	0.832%
3	8.372	849	857	864	rBV	1405739	2277469	1.59%	0.587%
4	10.299	1177	1185	1195	rVB	1050533	1838190	1.28%	0.474%
5	13.331	1695	1701	1708	rVB	987768	1584664	1.11%	0.409%
6	14.042	1799	1822	1824	rBV3	27724072	143349961	100.00%	36.967%
7	15.487	2063	2068	2073	rBV3	1232030	2209248	1.54%	0.570%
8	16.428	2225	2228	2233	rVB2	2988060	4280501	2.99%	1.104%
9	18.478	2571	2577	2594	rVB2	9276853	25401331	17.72%	6.550%
10	19.118	2682	2686	2696	rVB2	7698859	15653124	10.92%	4.037%
11	19.712	2783	2787	2802	rVB	8293817	17025657	11.88%	4.391%
12	20.123	2849	2857	2873	rVB2	17830116	39605396	27.63%	10.213%
13	20.628	2938	2943	2955	rVB	13630992	23538167	16.42%	6.070%
14	21.099	3019	3023	3026	rBV	7756029	12075845	8.42%	3.114%
15	21.128	3026	3028	3055	rVB	8360579	18850477	13.15%	4.861%
16	21.527	3088	3096	3109	rBV	11401175	23369009	16.30%	6.026%
17	22.097	3184	3193	3207	rBV	7184390	17634428	12.30%	4.548%
18	22.726	3292	3300	3316	rBV	3306818	10534517	7.35%	2.717%
19	23.255	3381	3390	3410	rBV	3876401	12006679	8.38%	3.096%
20	24.060	3520	3527	3551	rVB2	1894920	7284811	5.08%	1.879%

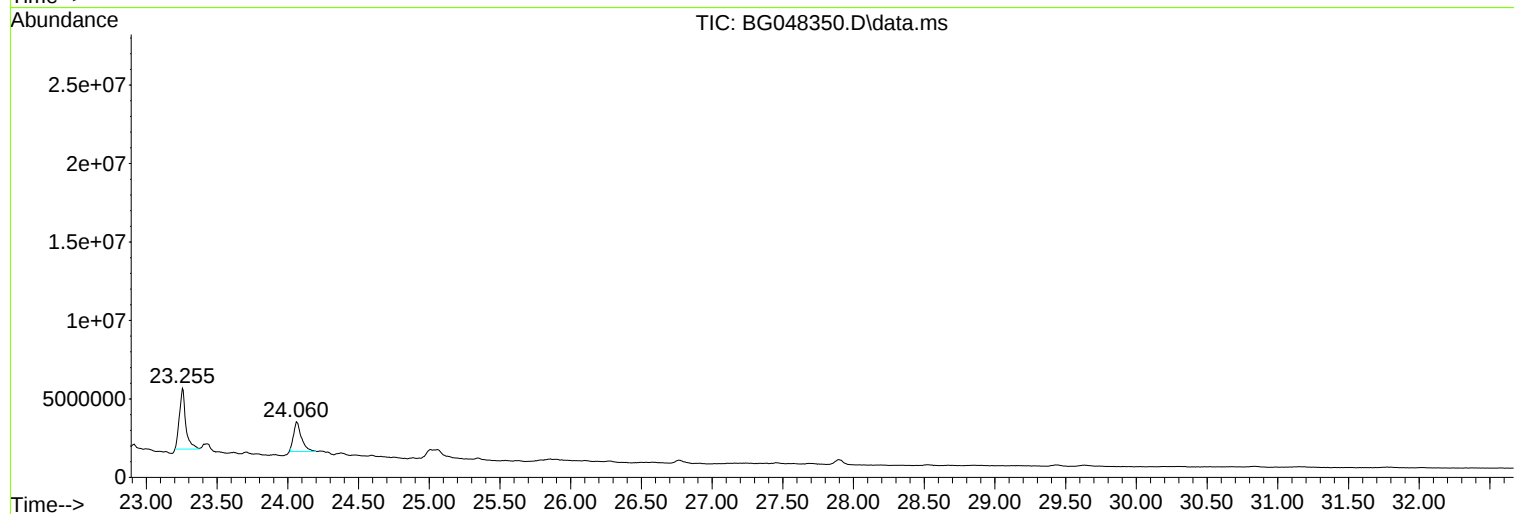
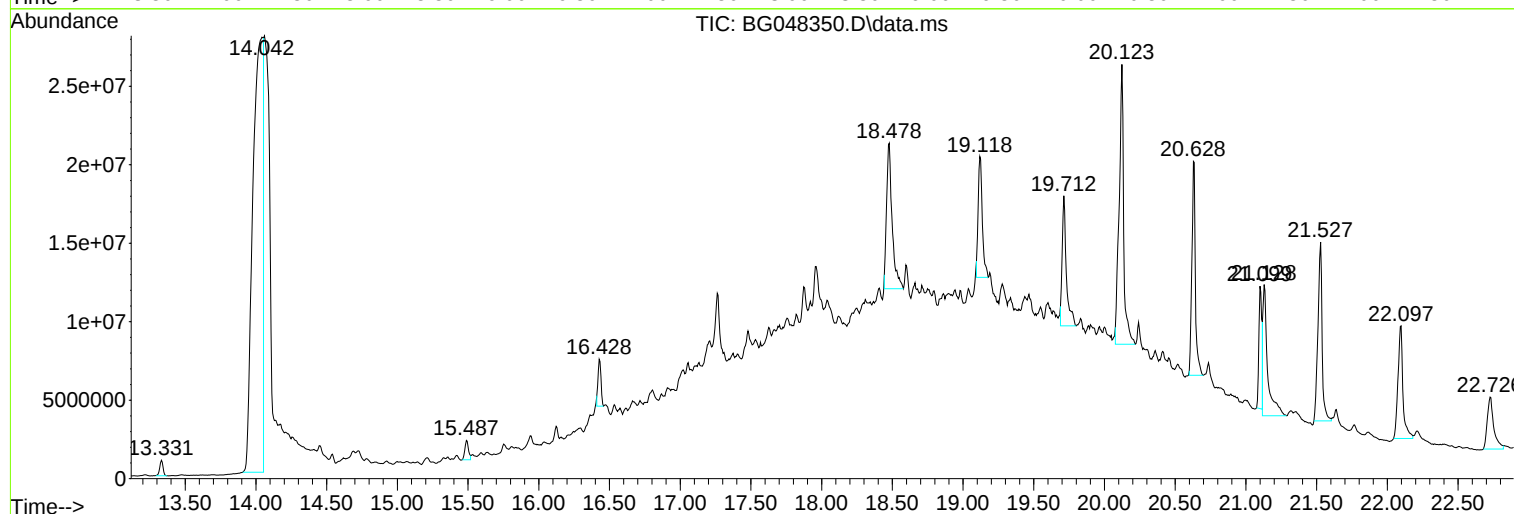
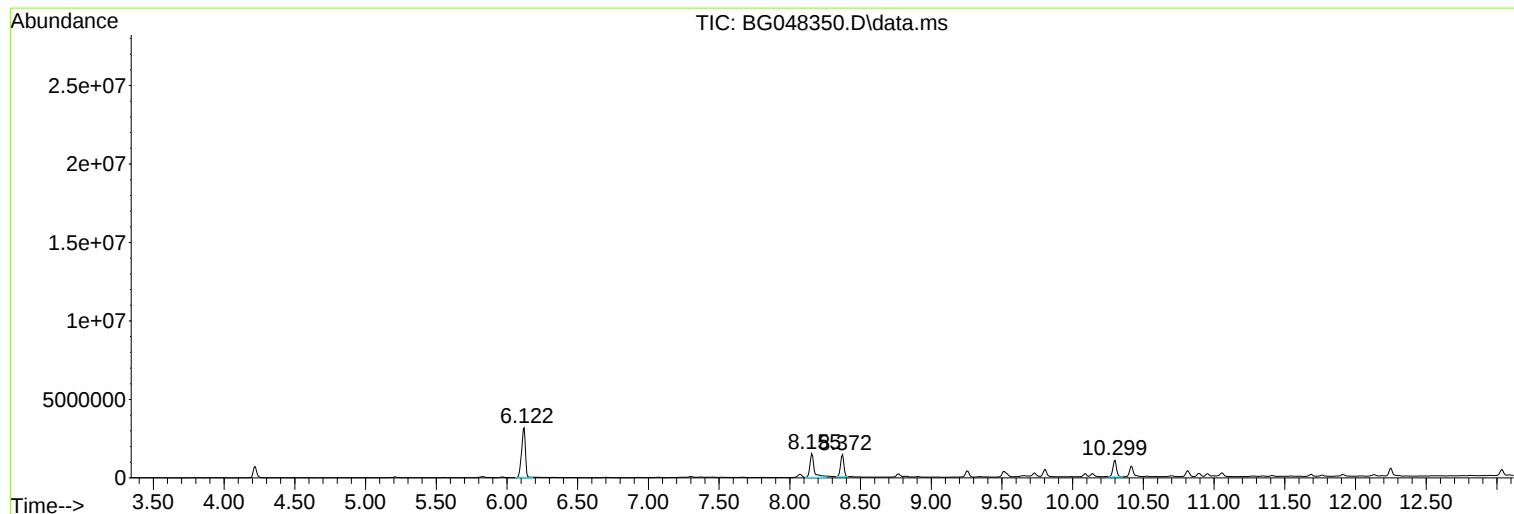
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
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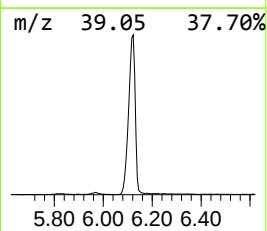
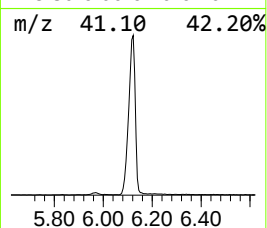
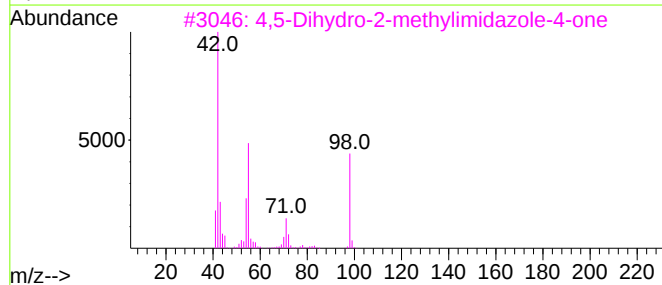
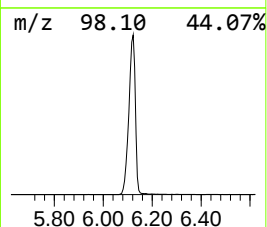
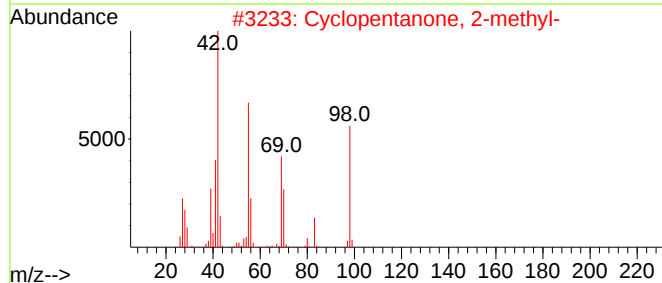
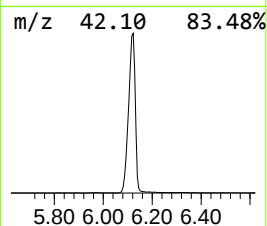
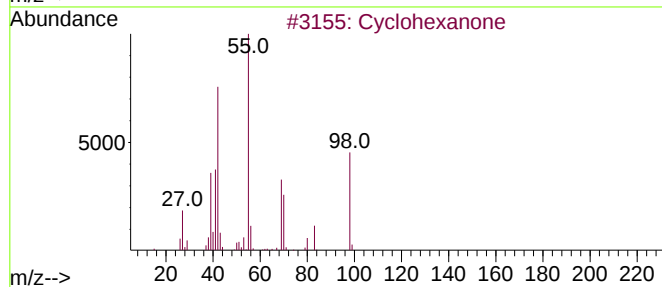
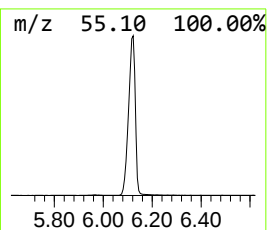
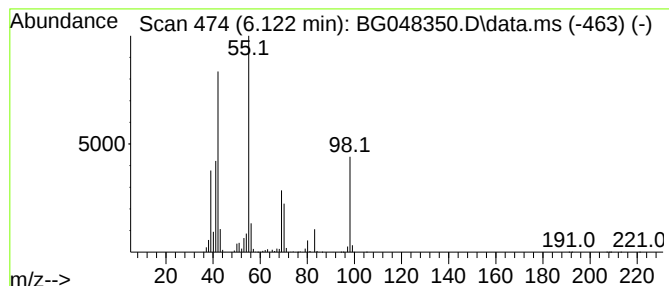
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.122	37.41 ng	6032960	1,4-Dichlorobenzene-d4	8.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	97
2			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	91
3			4,5-Dihydro-2-methylimidazole-4-one	98	C4H6N2O	004915-81-5	50
4			1-Pentene	70	C5H10	000109-67-1	46
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	46



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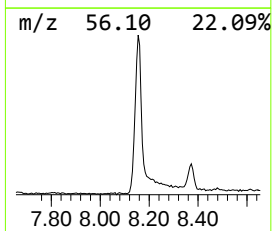
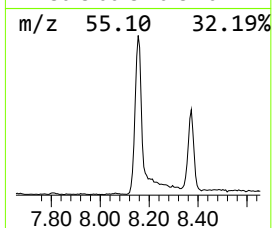
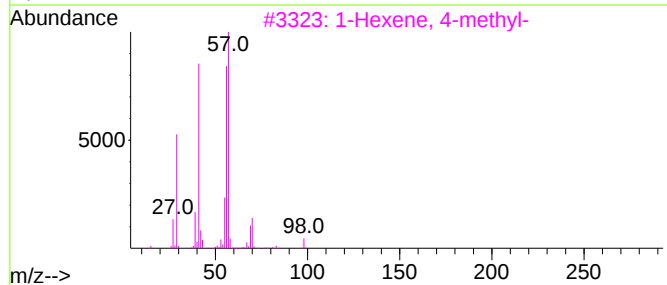
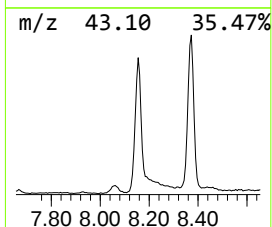
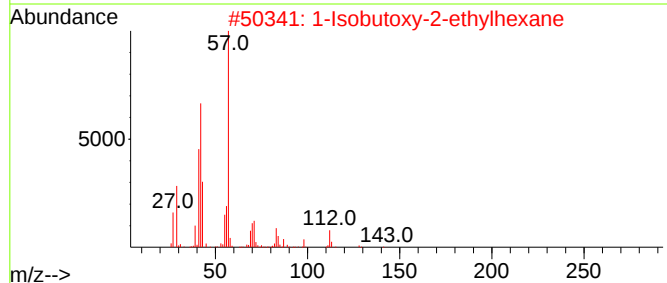
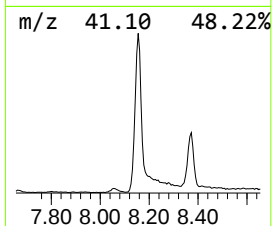
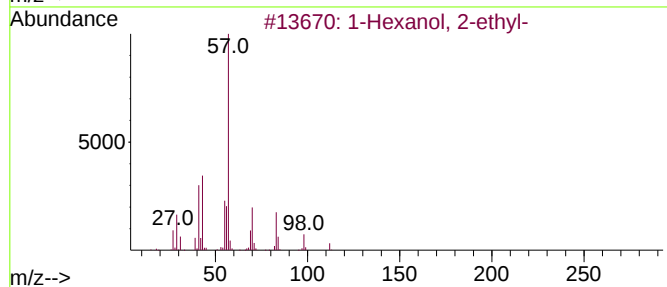
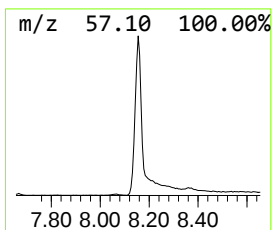
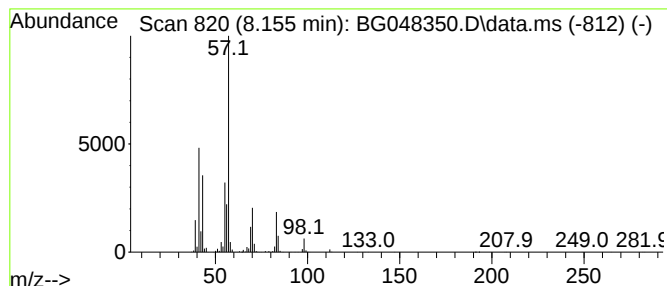
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.155	20.00 ng	3225100	1,4-Dichlorobenzene-d4	8.073

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	72
3		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	50
4		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
5		2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	1000365-19-6	50



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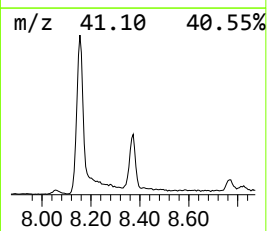
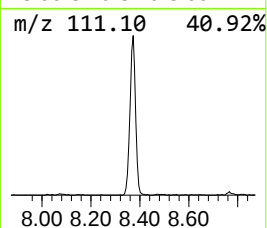
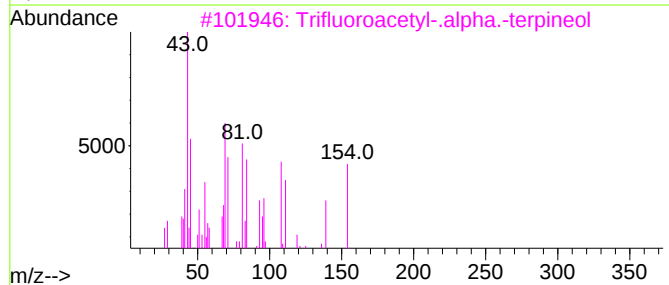
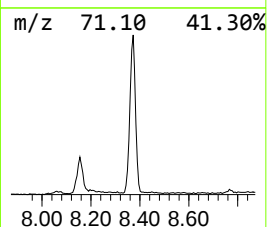
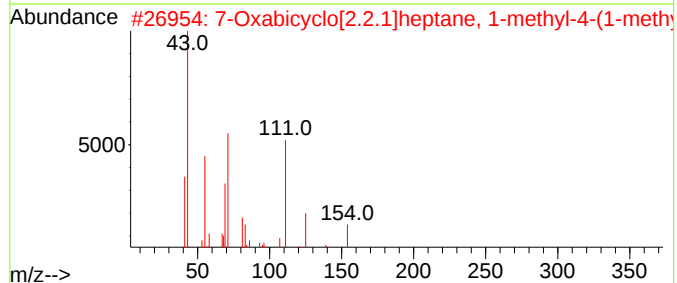
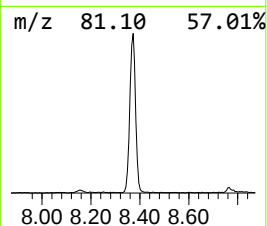
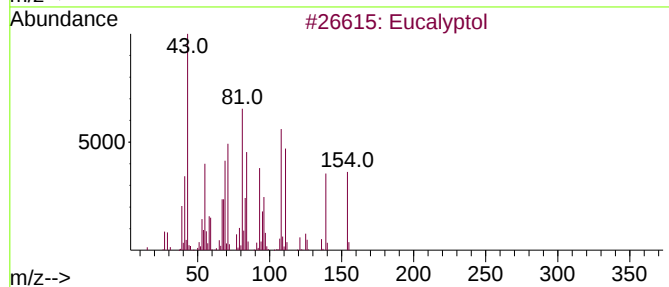
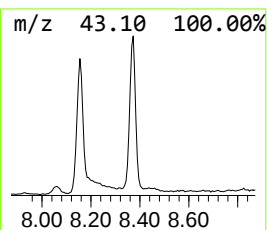
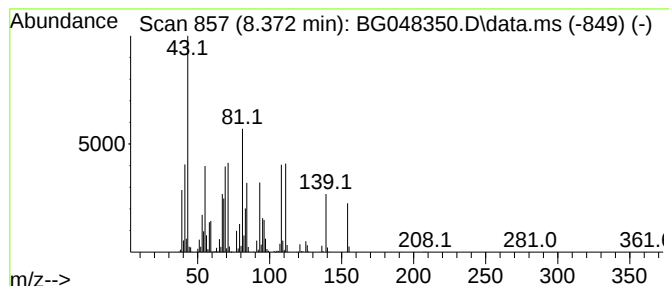
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Eucalyptol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.372	14.12 ng	2277470	1,4-Dichlorobenzene-d4	8.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	96
2			7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	37
3			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	37
4			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	25
5			2-Isopropyl-4-methylhex-2-enal	154	C10H18O	072668-37-2	14



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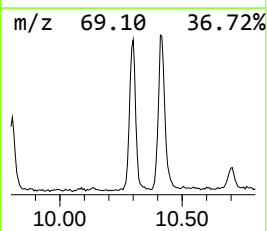
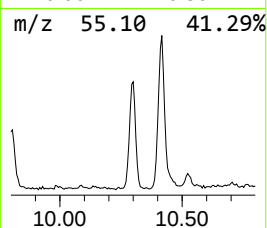
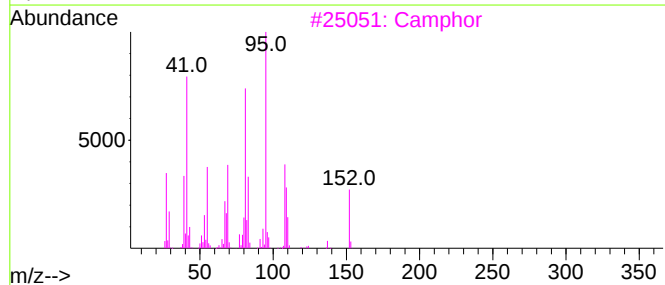
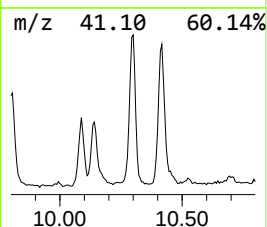
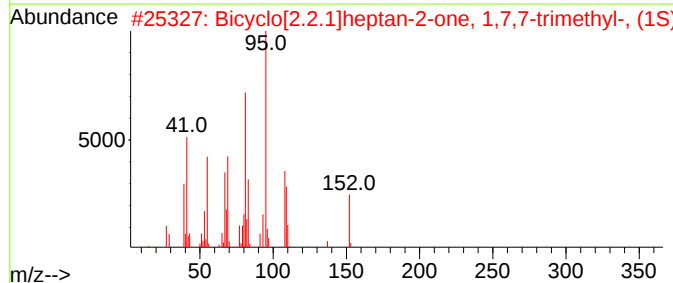
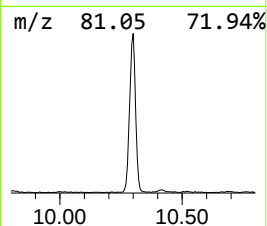
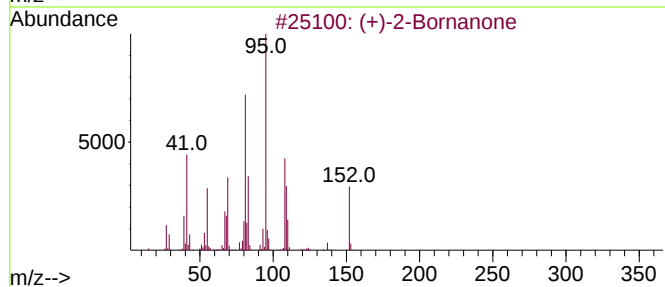
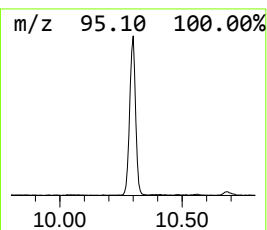
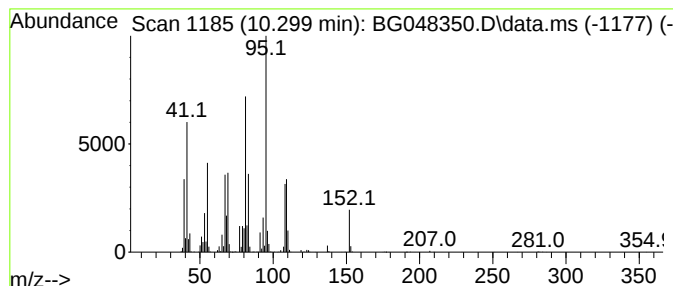
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 (+)-2-Bornanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.299	20.00 ng	1838190	Naphthalene-d8	10.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	96
2			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
3			Camphor	152	C10H16O	000076-22-2	94
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49
5			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	46



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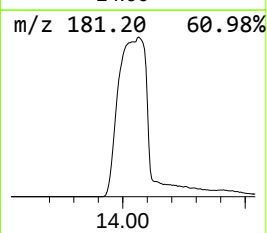
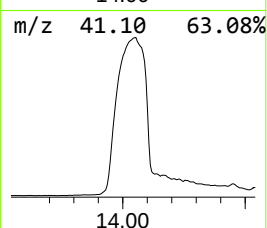
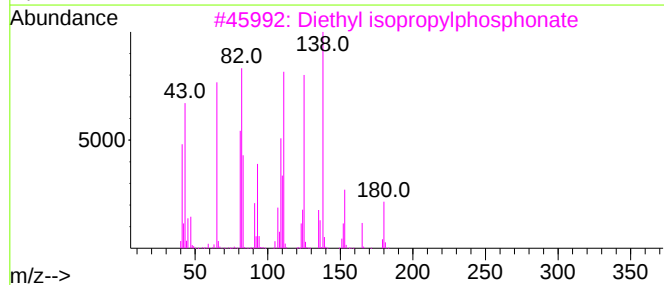
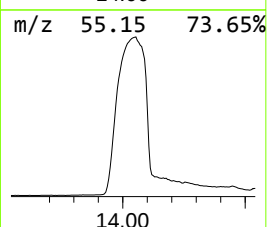
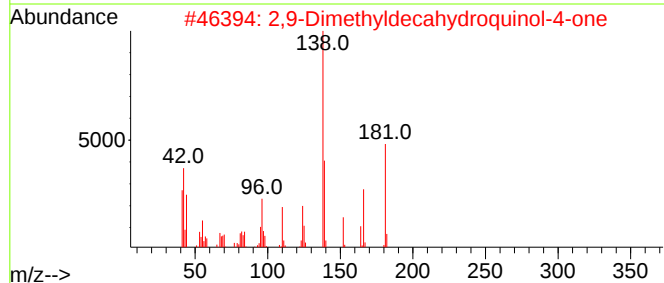
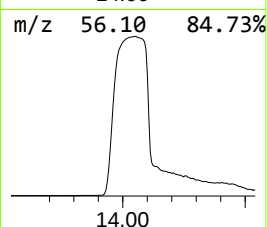
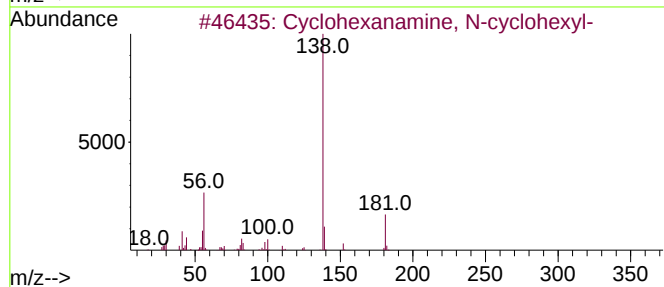
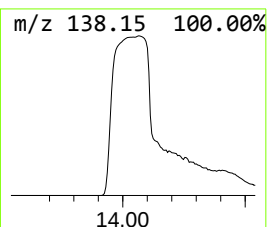
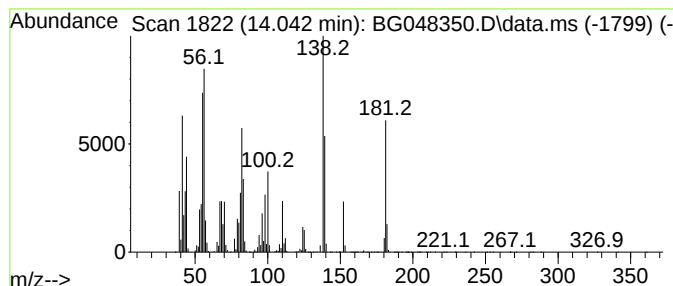
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexanamine, N-cyclohexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.042	20.00 ng	143350000	Acenaphthene-d10	14.724	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	52
2	2,9-Dimethyldecahydroquinol-4-one	181	C11H19NO	1000280-71-1	50
3	Diethyl isopropylphosphonate	180	C7H17O3P	001538-69-8	25
4	AI3-37135	181	C11H19NO	077251-49-1	18
5	2-Dimethylamino-6,7-dihydroimida...	181	C7H11N5O	144573-12-6	14



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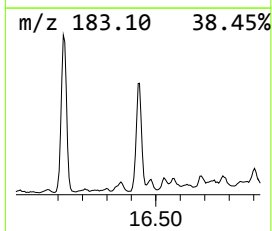
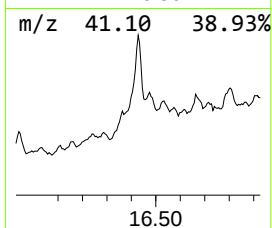
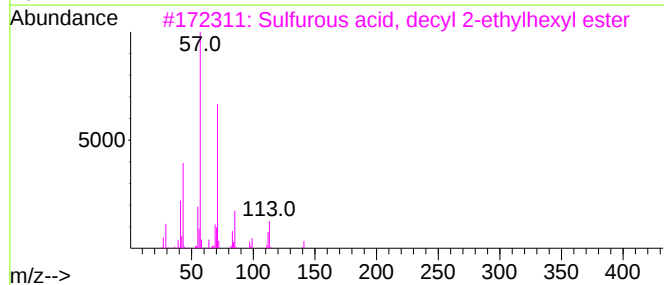
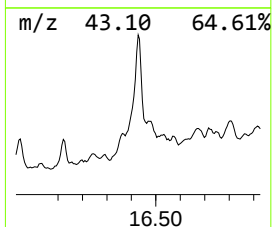
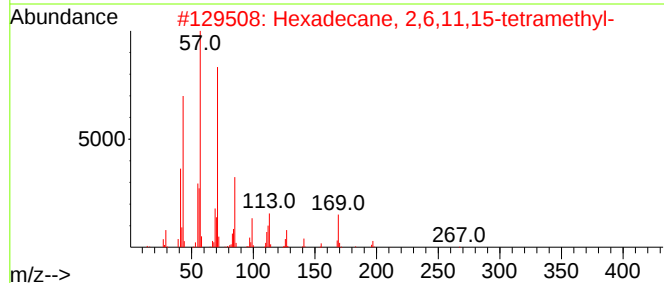
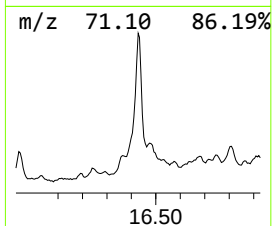
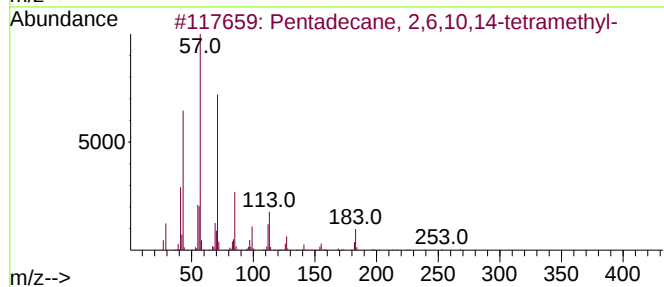
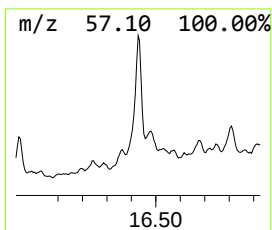
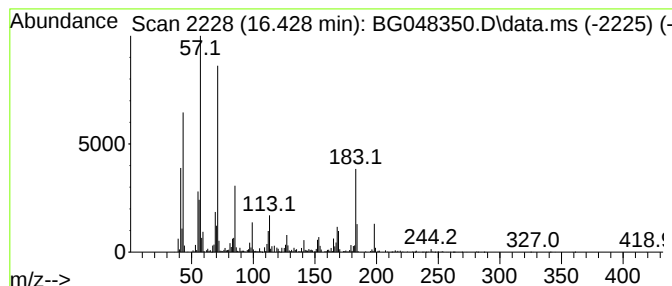
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BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecane, 2,6,10,14-tetr... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.427	3.37 ng	4280500	Phenanthrene-d10	17.485	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	58
2	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	58
3	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	53
4	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	52
5	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030521\
Data File : BG048350.D
Acq On : 5 Mar 2021 23:09
Operator : CG/JU
Sample : M1553-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

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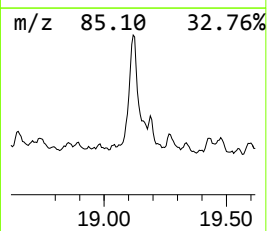
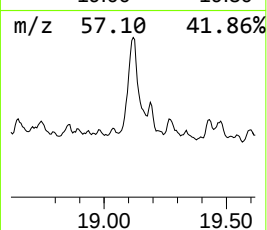
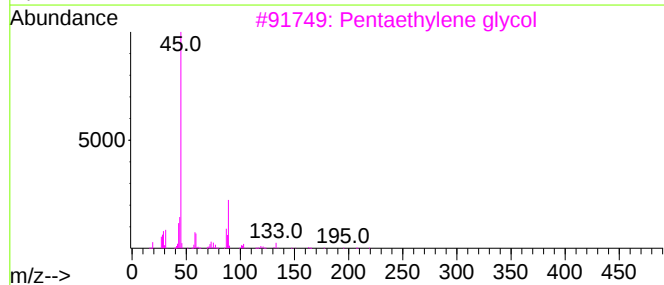
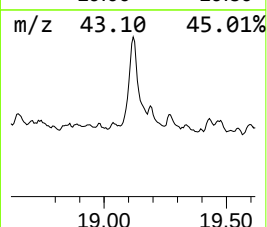
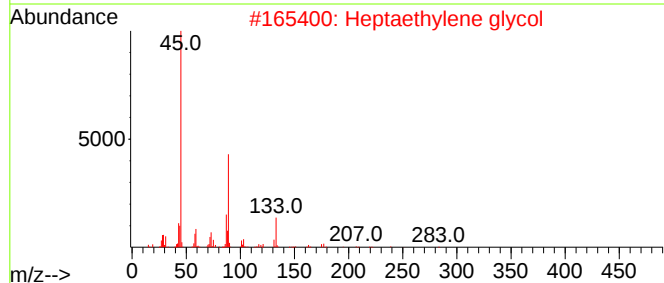
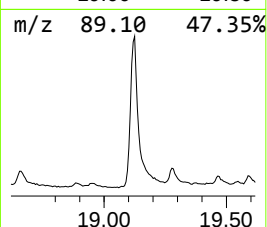
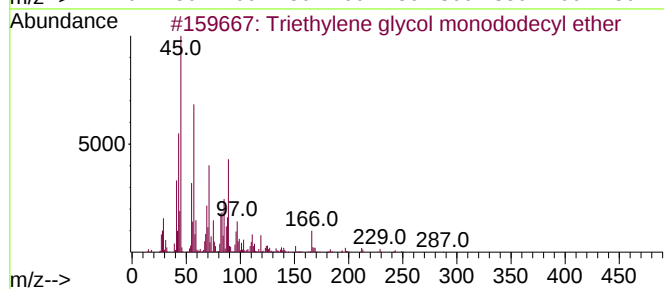
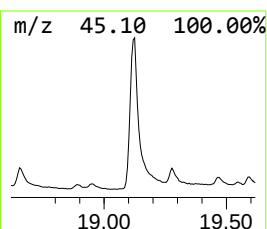
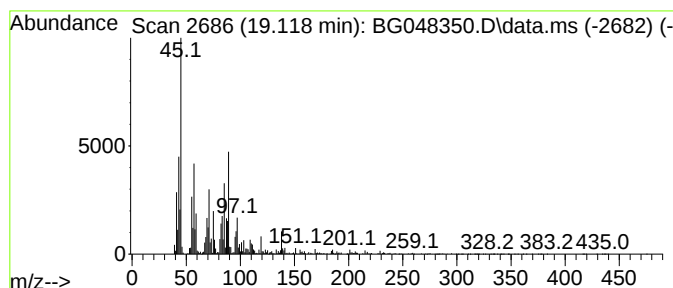
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triethylene glycol monododecyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.119	12.32 ng	15653100	Phenanthrene-d10	17.485

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triethylene glycol monododecyl e...	318	C18H38O4	003055-94-5	64
2			Heptaethylene glycol	326	C14H30O8	005617-32-3	49
3			Pentaethylene glycol	238	C10H22O6	004792-15-8	49
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	47
5			Hexaethylene glycol	282	C12H26O7	002615-15-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030521\
Data File : BG048350.D
Acq On : 5 Mar 2021 23:09
Operator : CG/JU
Sample : M1553-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

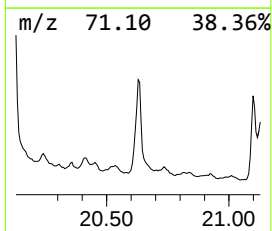
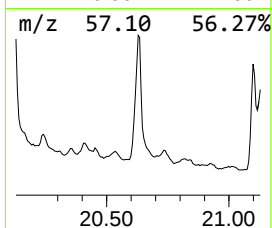
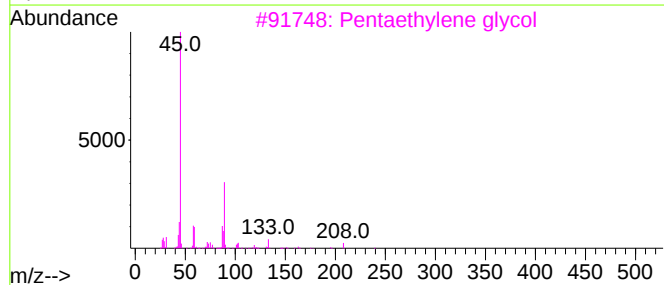
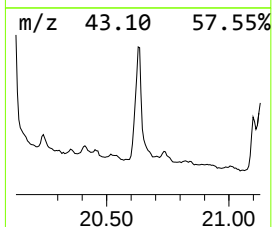
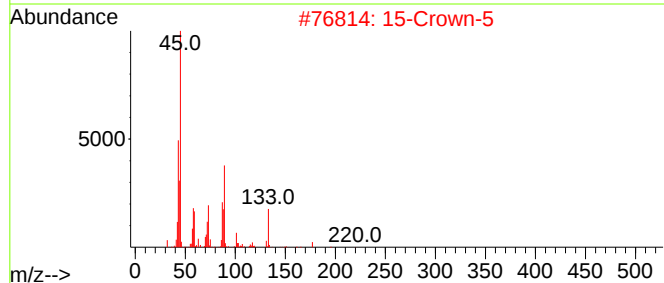
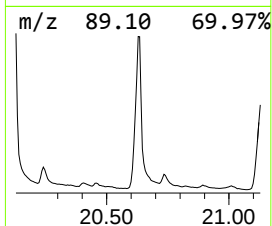
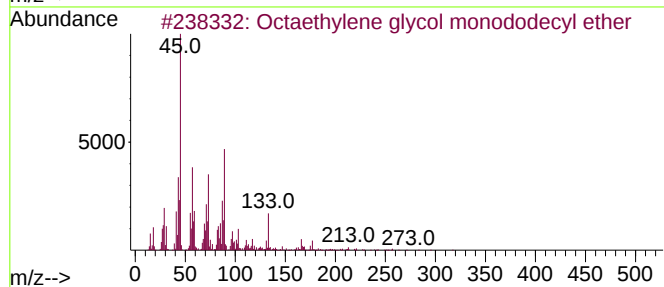
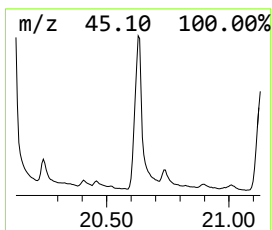
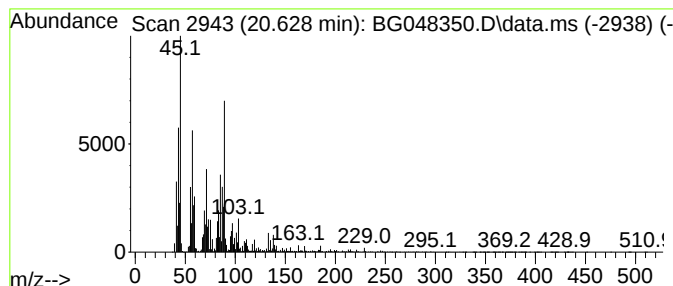
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octaethylene glycol monodod... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.628	20.14 ng	23538200	Chrysene-d12	21.768	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octaethylene glycol monododecyl ...	538	C28H58O9	003055-98-9	64
2	15-Crown-5	220	C10H20O5	033100-27-5	55
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	50
4	Methoxyacetic acid, 3-pentadecyl...	300	C18H36O3	1000282-05-2	46
5	Methyl pentadecyl ether	242	C16H34O	007307-52-0	44



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030521\
Data File : BG048350.D
Acq On : 5 Mar 2021 23:09
Operator : CG/JU
Sample : M1553-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

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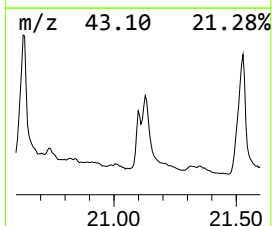
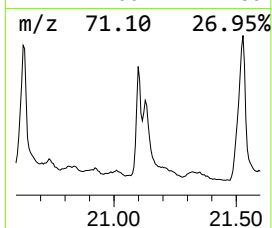
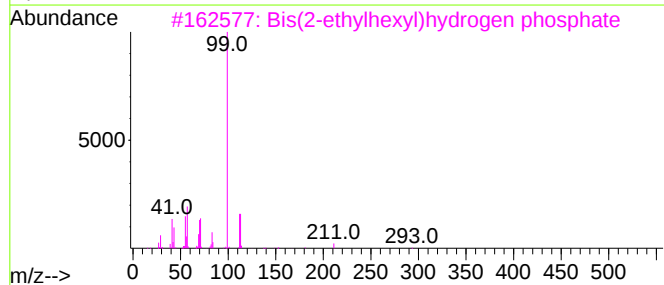
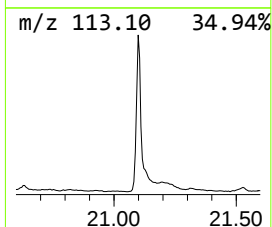
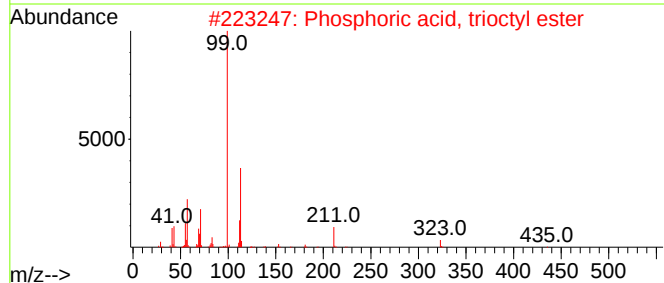
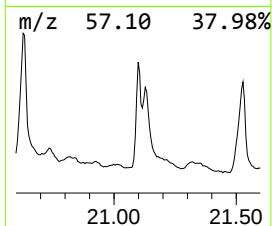
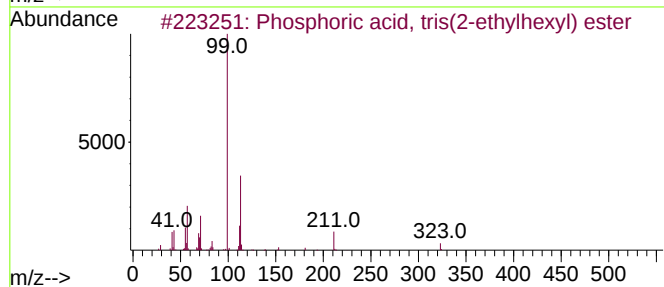
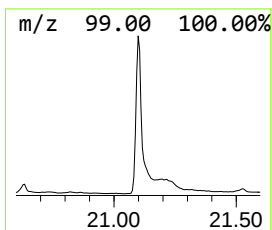
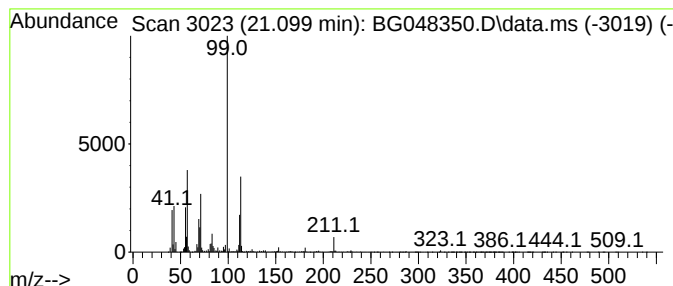
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phosphoric acid, tris(2-eth... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.099	10.33 ng	12075800	Chrysene-d12	21.768

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphoric acid, tris(2-ethylhex...	434	C24H51O4P	000078-42-2	72
2			Phosphoric acid, trioctyl ester	434	C24H51O4P	001806-54-8	72
3			Bis(2-ethylhexyl)hydrogen phosphate	322	C16H35O4P	000298-07-7	64
4			Hexanoic acid, cyclobutyl ester	170	C10H18O2	1000282-83-1	50
5			Hexanoic acid, 3-fluorophenyl ester	210	C12H15FO2	1000330-93-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030521\
Data File : BG048350.D
Acq On : 5 Mar 2021 23:09
Operator : CG/JU
Sample : M1553-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
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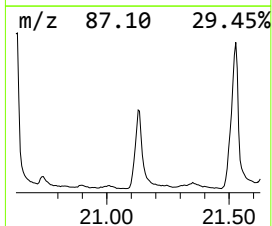
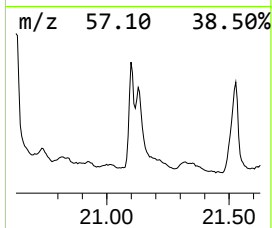
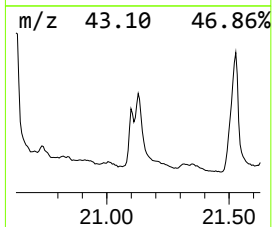
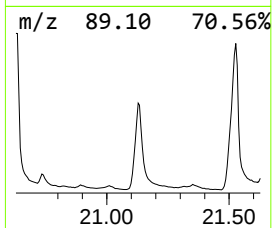
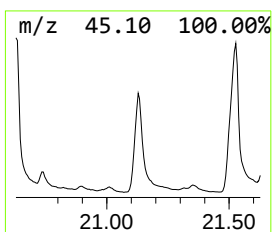
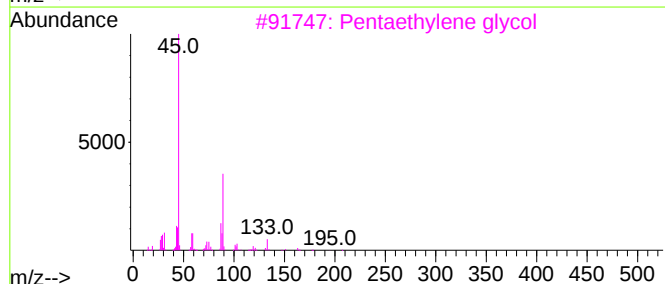
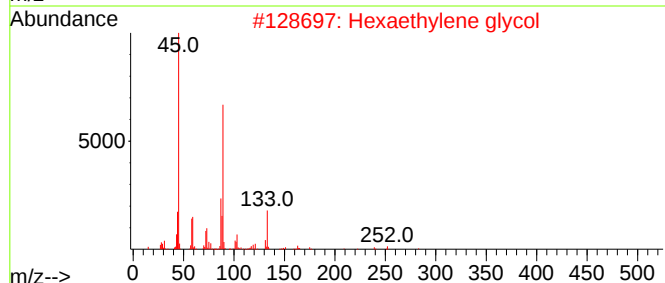
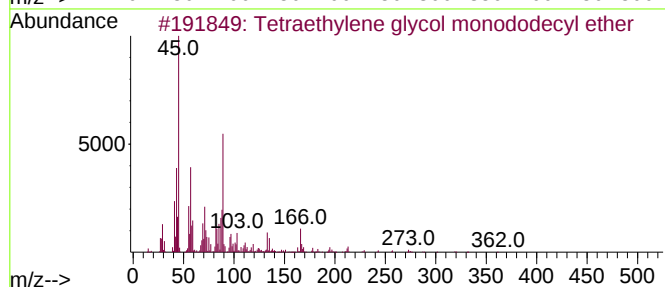
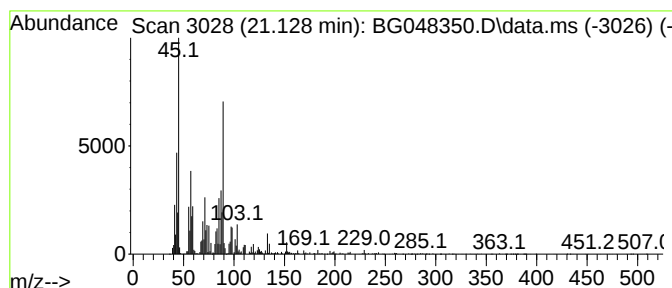
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetraethylene glycol monodo... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	16.13 ng	18850500	Chrysene-d12	21.768

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetraethylene glycol monododecyl...	362	C20H42O5	005274-68-0	72
2			Hexaethylene glycol	282	C12H26O7	002615-15-8	72
3			Pentaethylene glycol	238	C10H22O6	004792-15-8	64
4			2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	64
5			Heptaethylene glycol	326	C14H30O8	005617-32-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030521\
Data File : BG048350.D
Acq On : 5 Mar 2021 23:09
Operator : CG/JU
Sample : M1553-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

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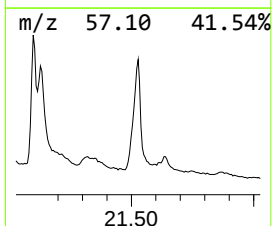
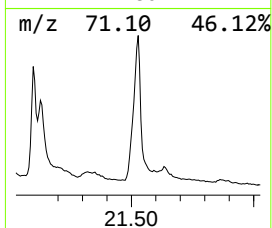
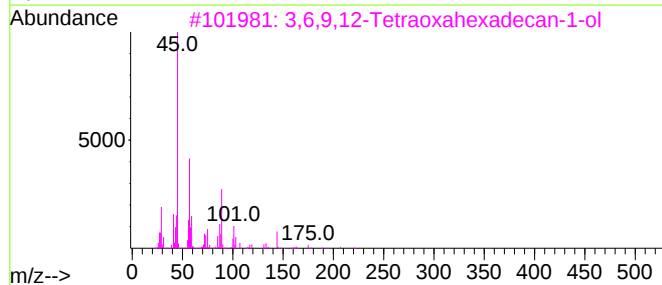
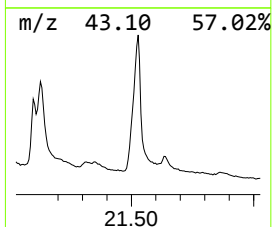
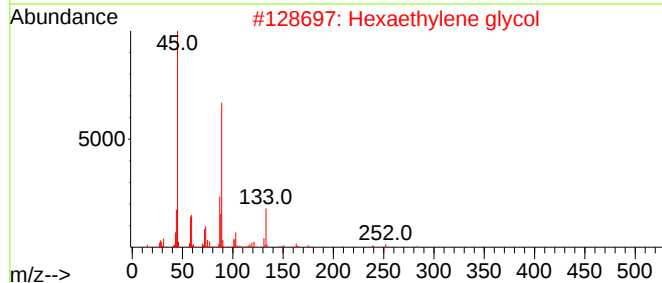
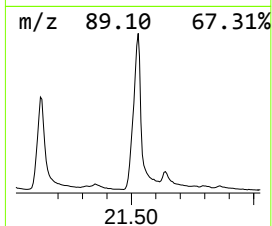
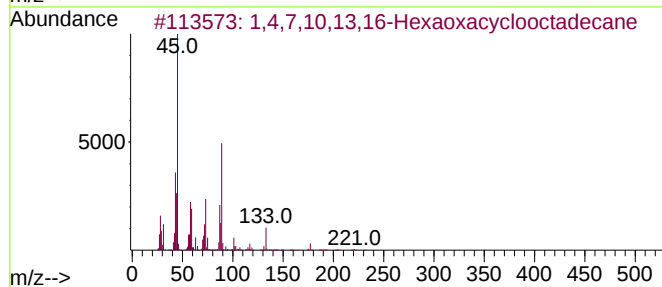
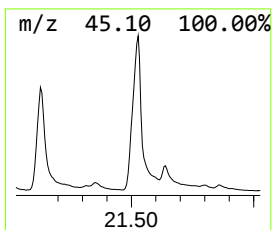
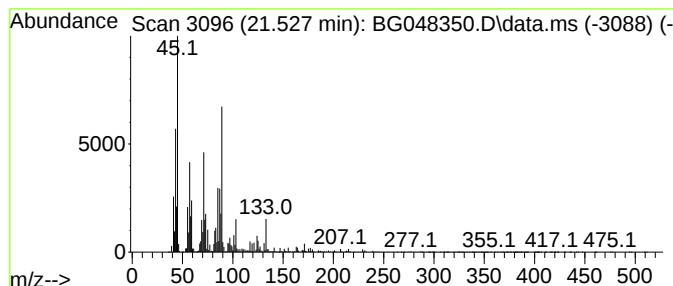
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1,4,7,10,13,16-Hexaoxacyclo... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.527	20.00 ng	23369000	Chrysene-d12	21.768

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	70		
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	62		
3	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	59		
4	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	58		
5	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	53		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030521\
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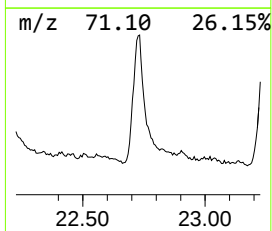
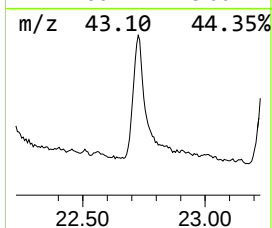
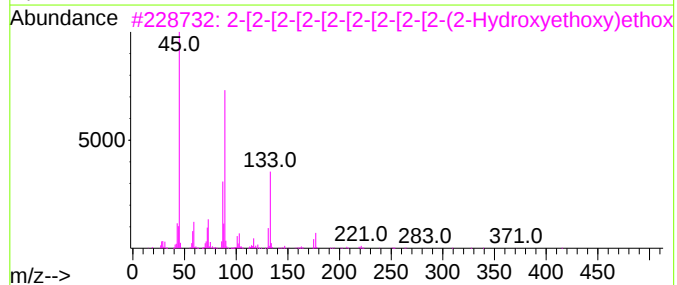
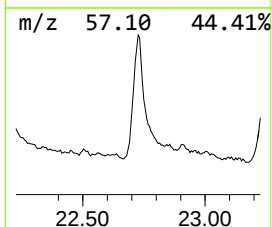
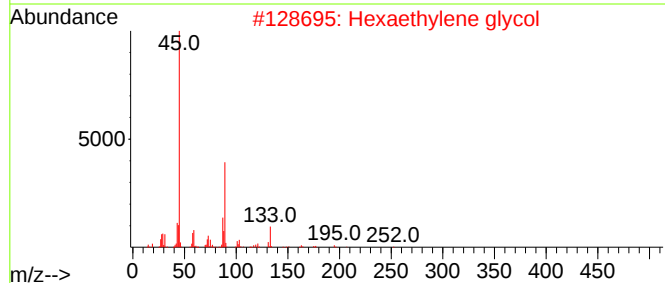
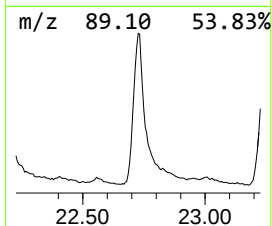
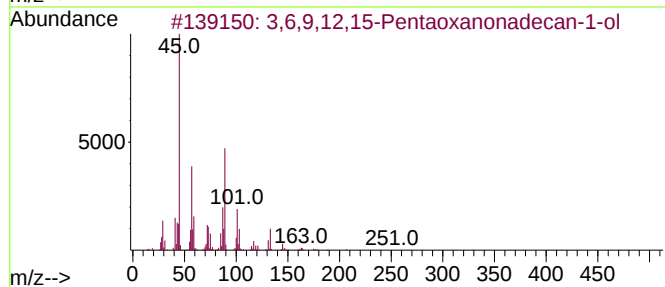
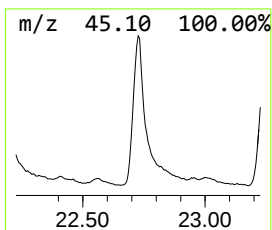
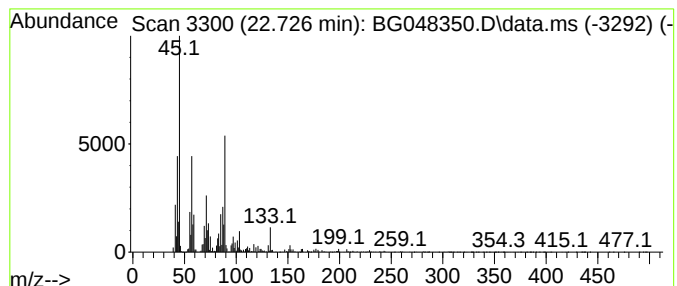
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.726	9.02 ng	10534500	Chrysene-d12	21.768	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	87
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	83
3	2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	80
4	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	80
5	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030521\
Data File : BG048350.D
Acq On : 5 Mar 2021 23:09
Operator : CG/JU
Sample : M1553-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
1729

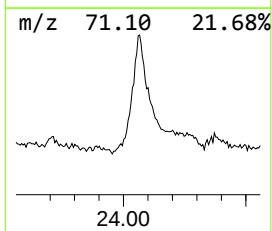
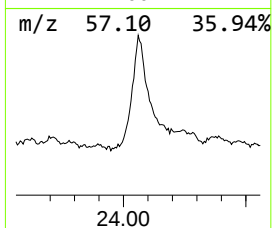
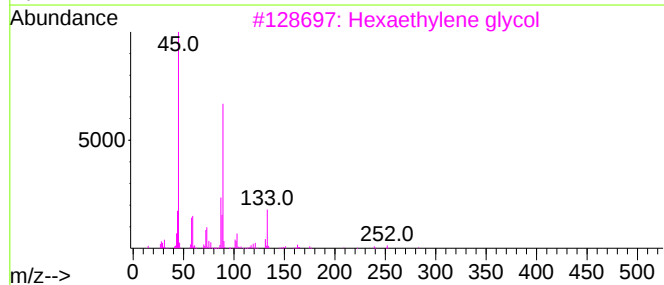
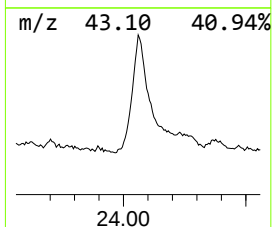
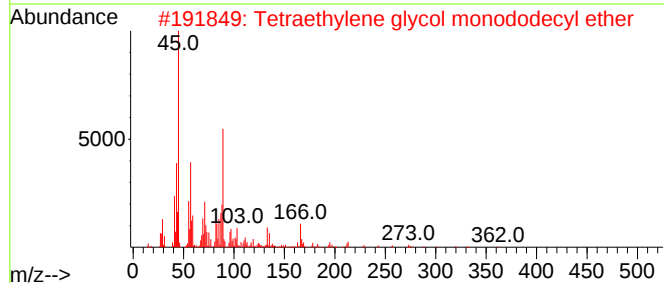
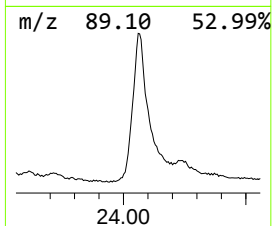
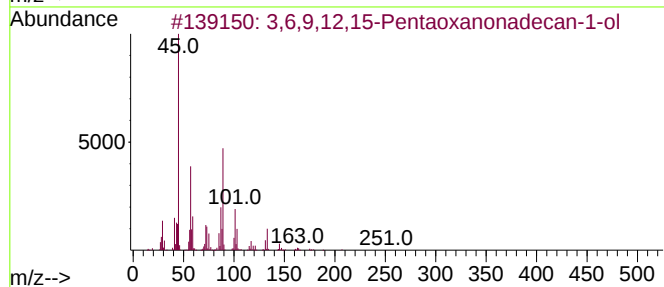
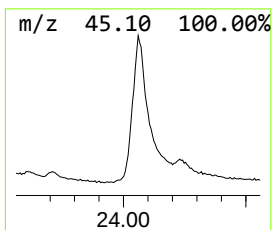
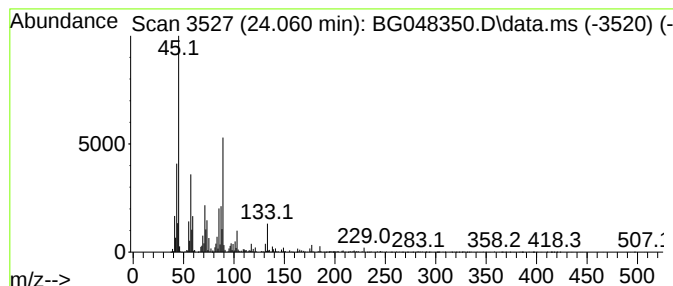
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Hexaethylene glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.060	20.00 ng	7284810	Perylene-d12	25.064

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	83		
2	Tetraethylene glycol monododecyl...	362	C20H42O5	005274-68-0	80		
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	74		
4	2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	74		
5	2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	74		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030521\
Data File : BG048350.D
Acq On : 5 Mar 2021 23:09
Operator : CG/JU
Sample : M1553-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1729

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexanone	6.122	37.4	ng	6032960	1	8.073	3225100	20.0
1-Hexanol, 2-et...	8.155	20.0	ng	3225100	1	8.073	3225100	20.0
Eucalyptol	8.372	14.1	ng	2277470	1	8.073	3225100	20.0
(+)-2-Bornanone	10.299	20.0	ng	1838190	2	10.893	1838190	20.0
Cyclohexanamine...	14.042	20.0	ng	143350000	3	14.724	143350000	20.0
Pentadecane, 2,...	16.427	3.4	ng	4280500	4	17.485	25401300	20.0
unknown18.478	18.478	20.0	ng	25401300	4	17.485	25401300	20.0
Triethylene gly...	19.119	12.3	ng	15653100	4	17.485	25401300	20.0
Pentaethylene g...	19.712	14.6	ng	17025700	5	21.768	23369000	20.0
Octaethylene gl...	20.628	20.1	ng	23538200	5	21.768	23369000	20.0
Phosphoric acid...	21.099	10.3	ng	12075800	5	21.768	23369000	20.0
Tetraethylene g...	21.128	16.1	ng	18850500	5	21.768	23369000	20.0
1,4,7,10,13,16-...	21.527	20.0	ng	23369000	5	21.768	23369000	20.0
2-[2-[2-[2-[2-...	22.097	15.1	ng	17634400	5	21.768	23369000	20.0
3,6,9,12,15-Pen...	22.726	9.0	ng	10534500	5	21.768	23369000	20.0
3,6,9,12-Tetrao...	23.255	10.3	ng	12006700	5	21.768	23369000	20.0
Hexaethylene gl...	24.060	20.0	ng	7284810	6	25.064	7284810	20.0