

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
 Data File : BM029029.D
 Acq On : 08 Mar 2021 21:21
 Operator : CG/JU
 Sample : M1582-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 VEOLIA-72-11991

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_M\Methods\8270-BM022321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.363	60	64	79	rBV	62736	83394	32.96%	3.661%
2	5.246	379	384	394	rBB	145941	201740	79.73%	8.856%
3	6.869	654	660	670	rBV	132463	204922	80.99%	8.995%
4	7.669	791	796	802	rBB	40443	57795	22.84%	2.537%
5	8.845	990	996	1005	rBV	81422	129882	51.33%	5.701%
6	10.463	1265	1271	1278	rBV	47690	75195	29.72%	3.301%
7	12.951	1688	1694	1700	rBB	156448	213761	84.48%	9.383%
8	13.286	1746	1751	1765	rBB	9341	20079	7.94%	0.881%
9	13.804	1833	1839	1843	rBB	3283	4286	1.69%	0.188%
10	14.221	1904	1910	1917	rBV3	3901	9793	3.87%	0.430%
11	14.339	1924	1930	1935	rVB	66596	92791	36.67%	4.073%
12	15.833	2179	2184	2192	rBB	141097	189353	74.83%	8.312%
13	16.757	2337	2341	2348	rBV	3457	6104	2.41%	0.268%
14	17.080	2391	2396	2402	rBV	75845	104109	41.14%	4.570%
15	17.980	2544	2549	2556	rBV	21664	28666	11.33%	1.258%
16	18.751	2672	2680	2689	rBV	14611	24426	9.65%	1.072%
17	19.139	2743	2746	2752	rVB	5143	6231	2.46%	0.274%
18	19.262	2762	2767	2777	rBV2	9747	14077	5.56%	0.618%
19	19.504	2804	2808	2812	rVB	4618	5901	2.33%	0.259%
20	19.709	2838	2843	2848	rVB	221789	253032	100.00%	11.107%
21	20.321	2943	2947	2957	rBV	42246	62063	24.53%	2.724%
22	20.974	3053	3058	3065	rBV	31631	43101	17.03%	1.892%
23	21.256	3101	3106	3111	rBV	103625	129562	51.20%	5.687%
24	21.592	3159	3163	3176	rBV	66517	115100	45.49%	5.052%
25	22.892	3380	3384	3394	rBV	39887	76563	30.26%	3.361%
26	23.415	3468	3473	3479	rVB2	72963	126188	49.87%	5.539%

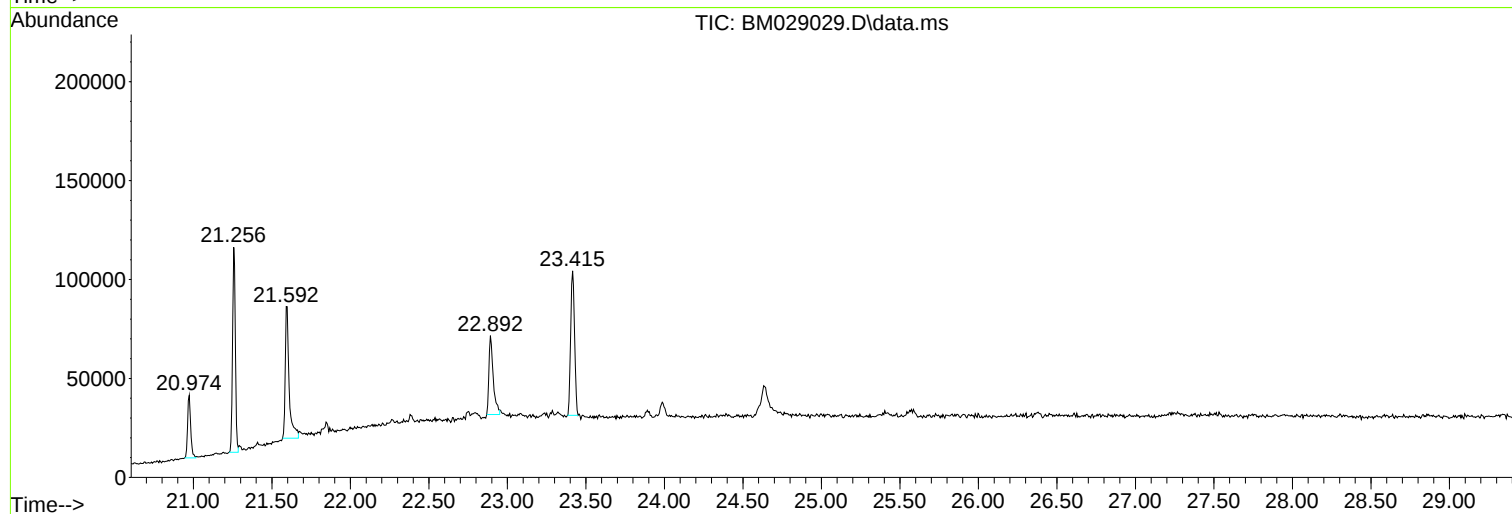
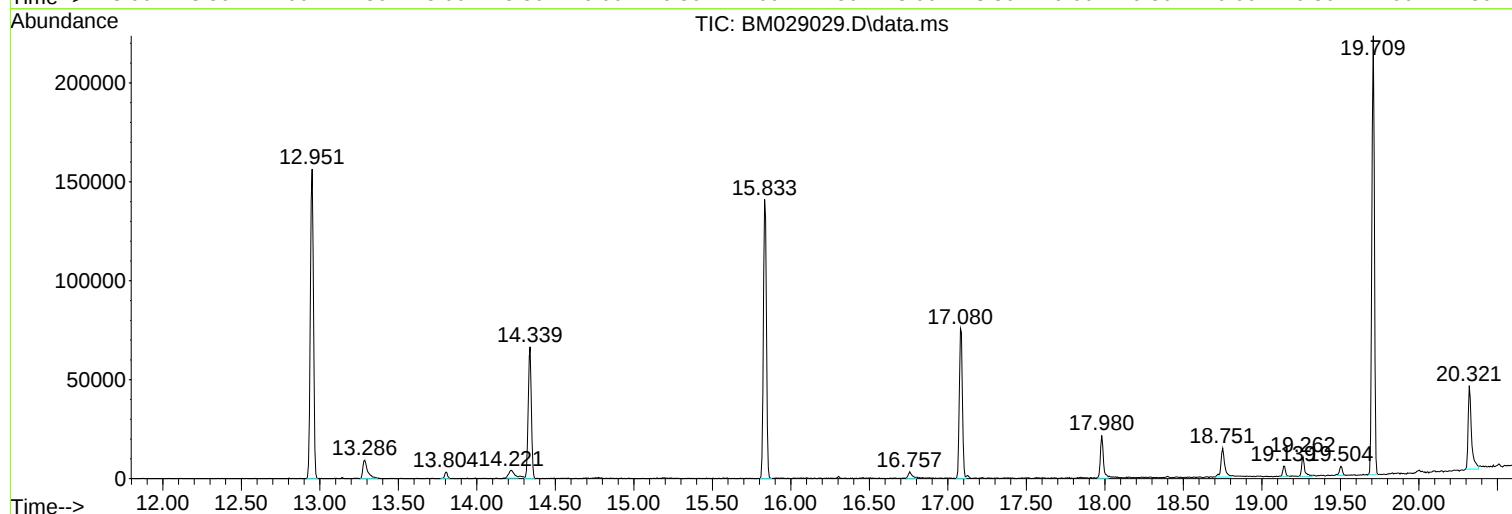
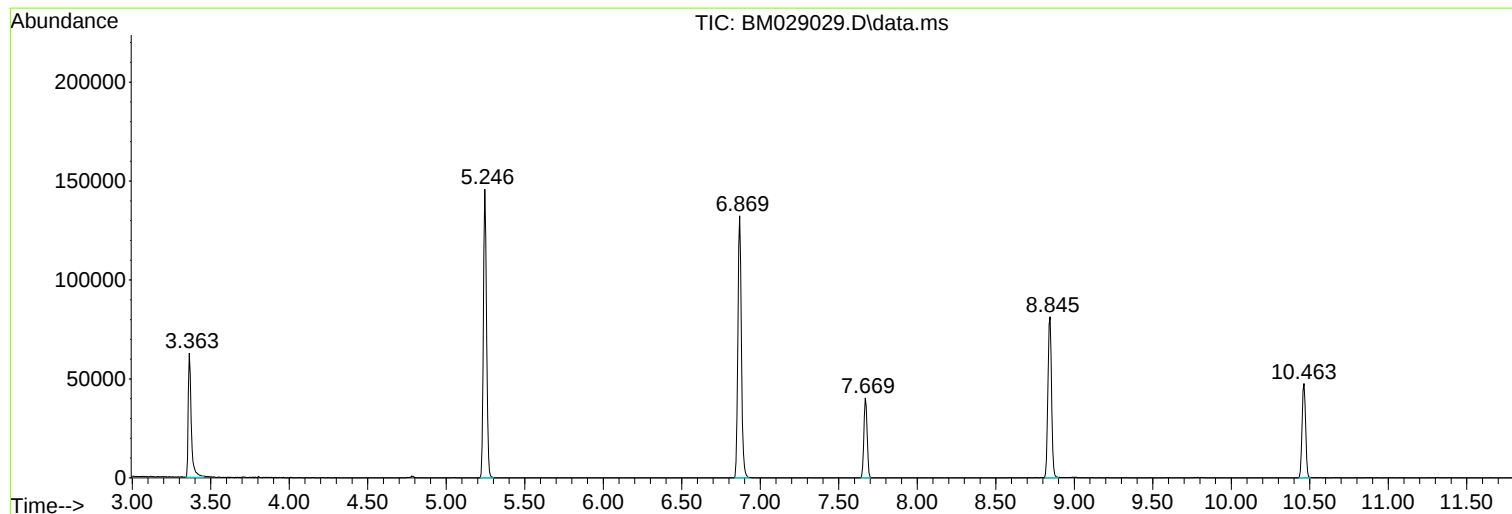
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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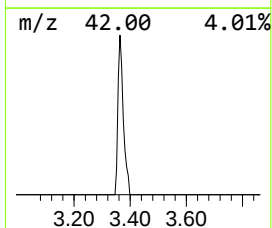
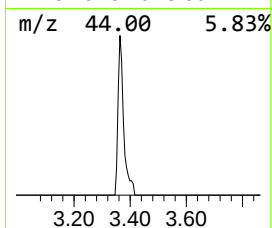
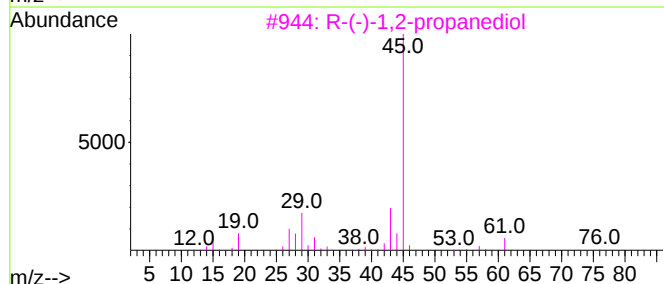
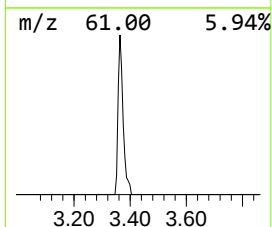
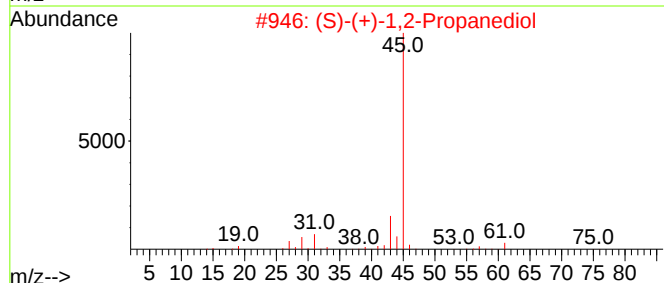
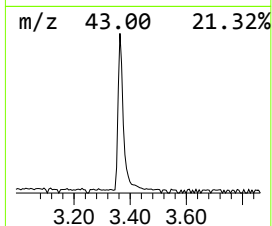
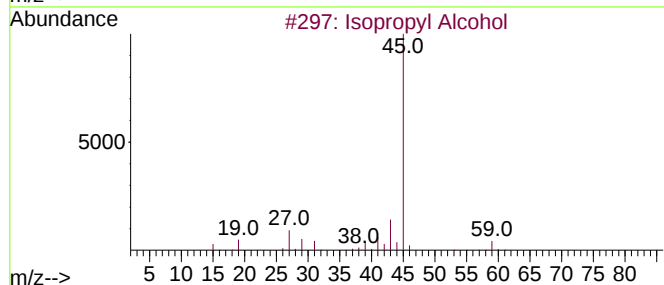
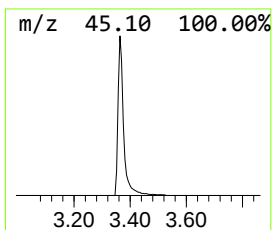
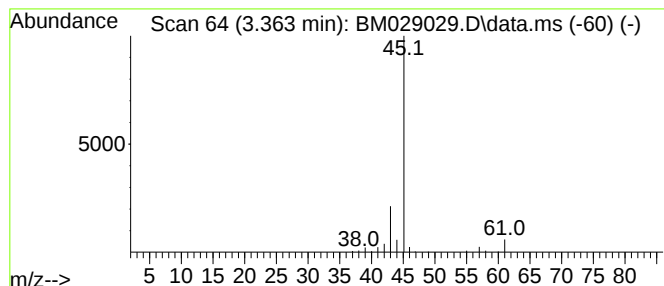
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	28.86 ng	83394	1,4-Dichlorobenzene-d4	7.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	80
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4			Propylene Glycol	76	C3H8O2	000057-55-6	43
5			Formamide	45	CH3NO	000075-12-7	5



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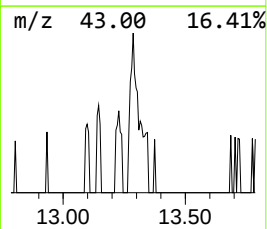
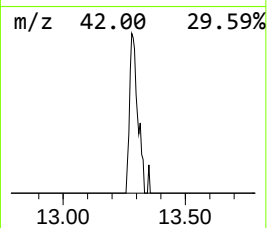
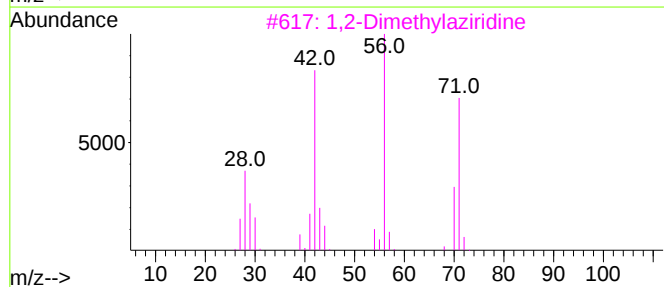
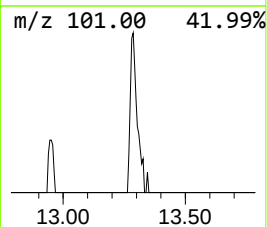
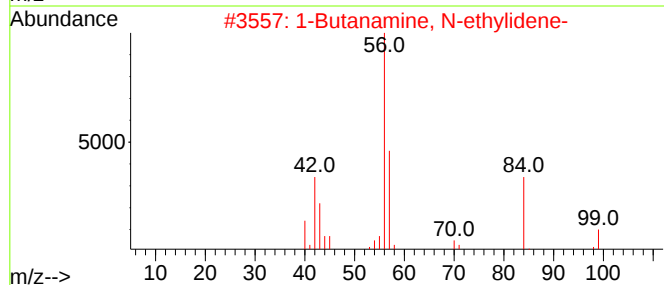
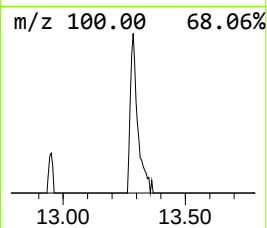
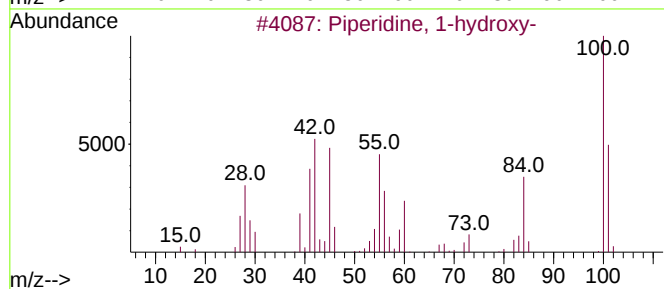
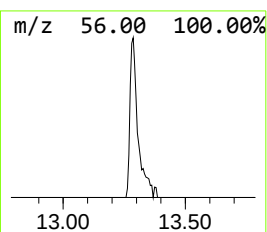
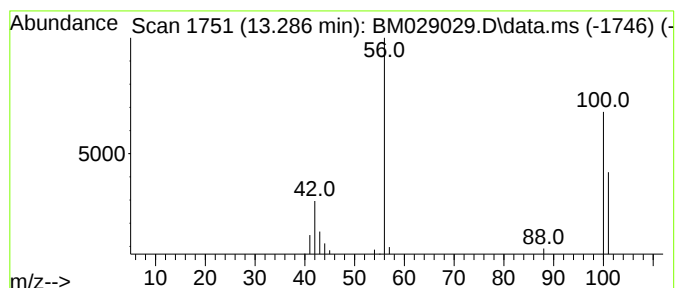
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown13.286 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	4.33 ng	20079	Acenaphthene-d10	14.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	32
2			1-Butanamine, N-ethylidene-	99	C6H13N	006898-74-4	23
3			1,2-Dimethylaziridine	71	C4H9N	030757-96-1	17
4			2-Piperazinone	100	C4H8N2O	005625-67-2	12
5			2-Propanone, ethylhydrazone	100	C5H12N2	007422-99-3	10



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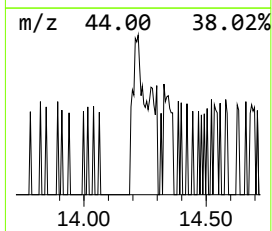
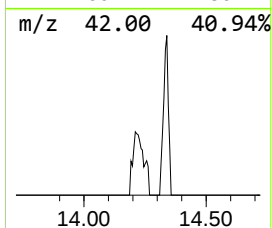
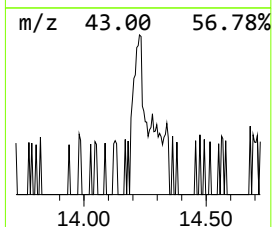
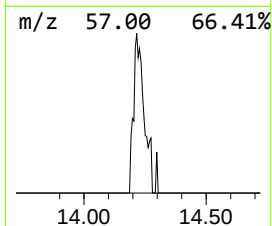
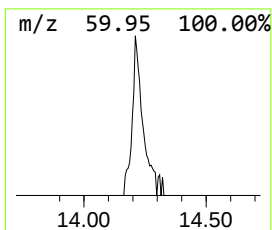
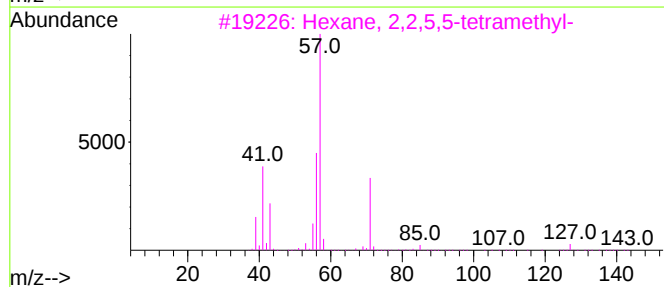
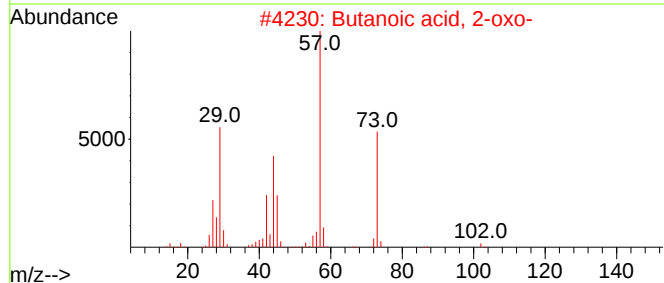
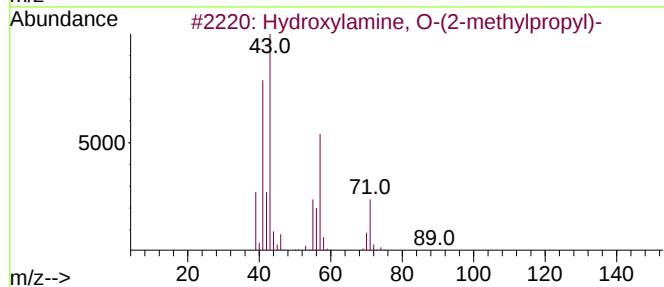
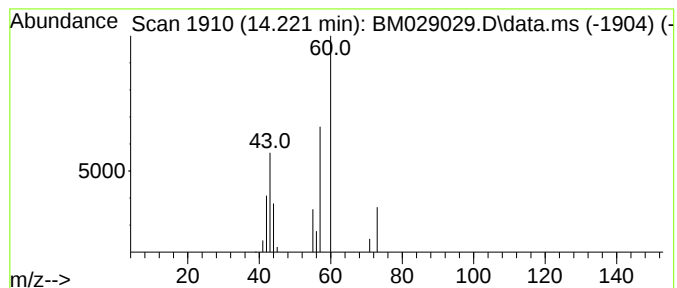
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown14.222 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.222	2.11 ng	9793	Acenaphthene-d10	14.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	12
2			Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	9
3			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	9
4			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	7
5			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	7



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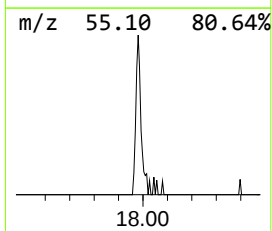
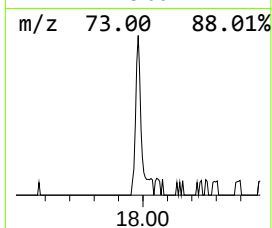
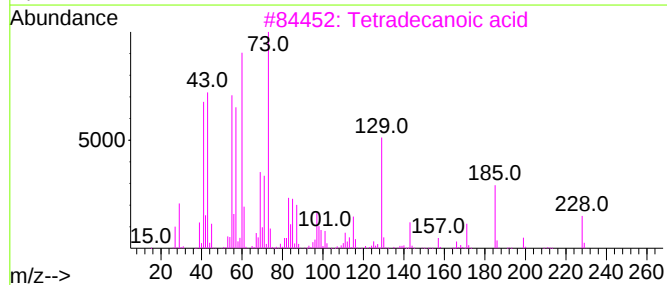
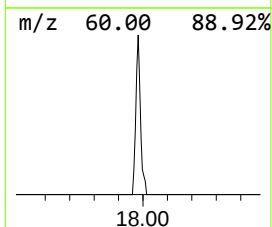
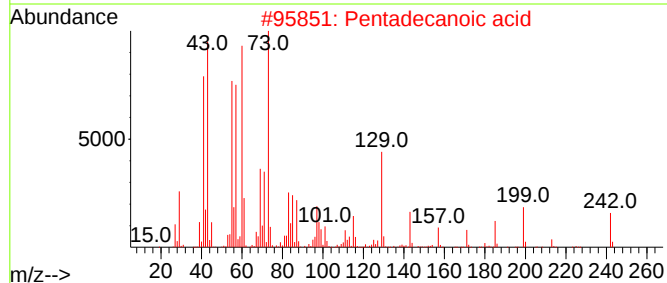
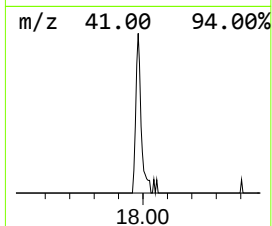
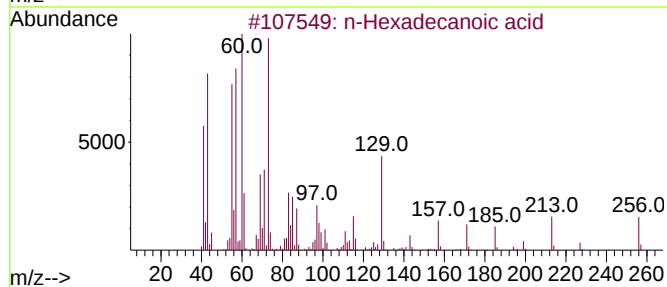
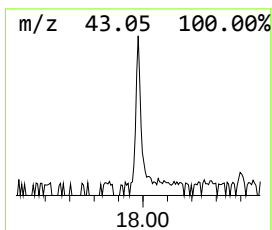
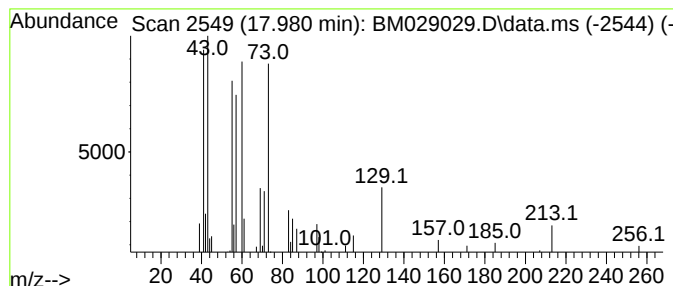
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	5.51 ng	28666	Phenanthrene-d10	17.080

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	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	64



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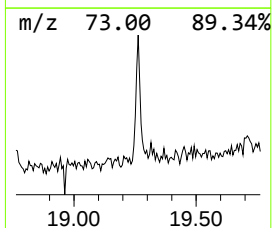
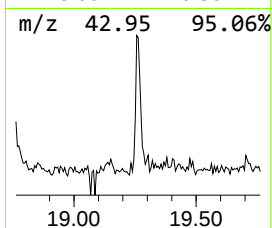
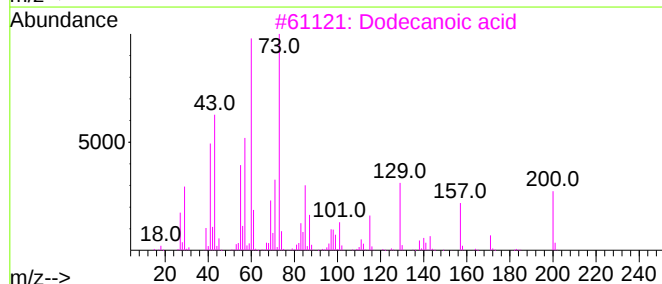
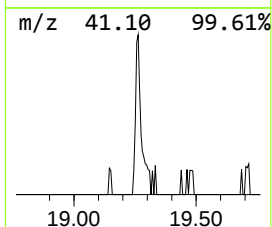
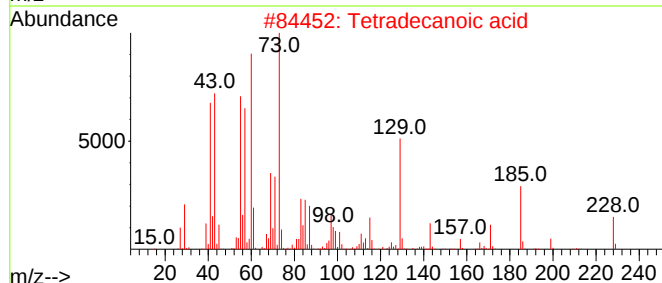
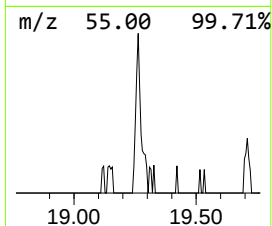
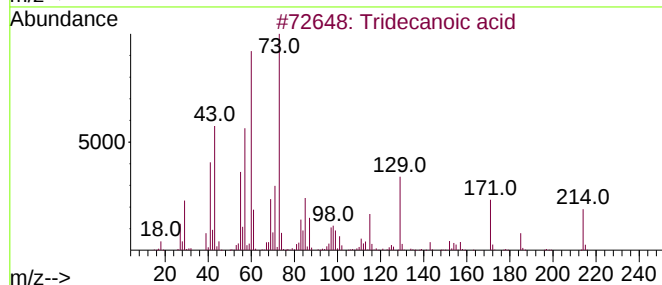
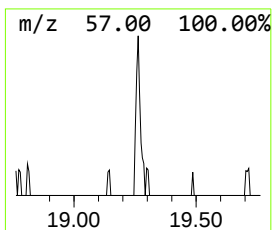
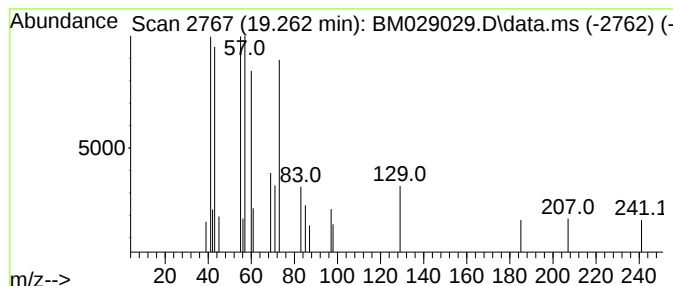
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Peak Number 6 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.262	2.17 ng	14077	Chrysene-d12	21.256

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	72
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		Dodecanoic acid	200	C12H24O2	000143-07-7	59
4		Trehalose	342	C12H22O11	000099-20-7	47
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



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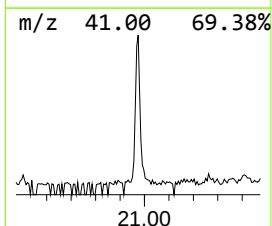
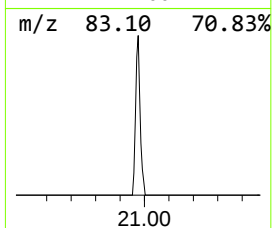
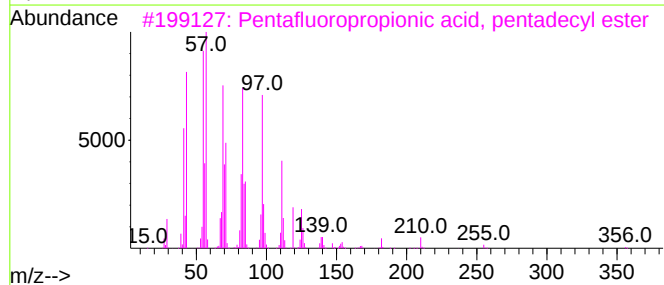
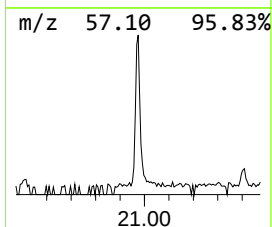
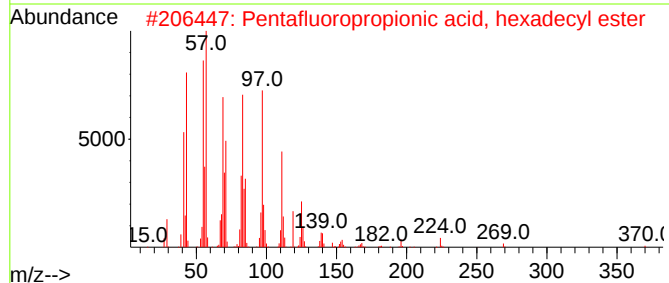
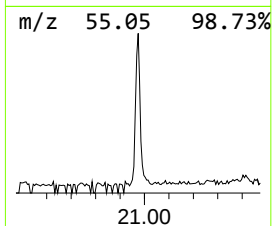
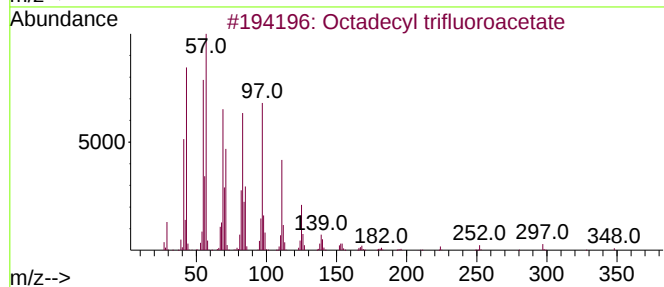
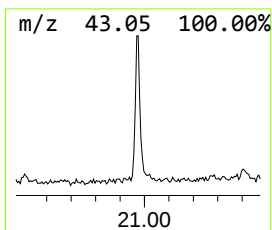
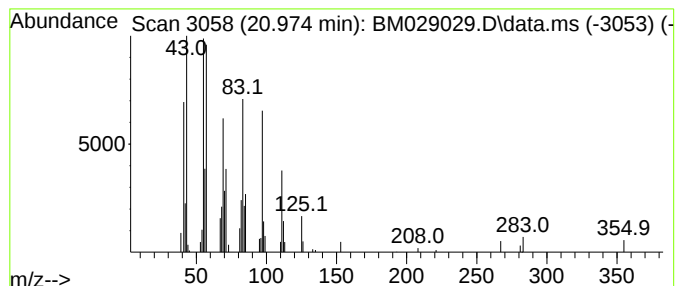
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	6.65 ng	43101	Chrysene-d12	21.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
2			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
3			Pentafluoropropionic acid, pentadecyl ester	374	C18H31F5O2	959092-08-1	91
4			1-Tricosene	322	C23H46	018835-32-0	91
5			Trichloroacetic acid, hexadecyl ester	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029029.D
Acq On : 08 Mar 2021 21:21
Operator : CG/JU
Sample : M1582-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VEOLIA-72-11991

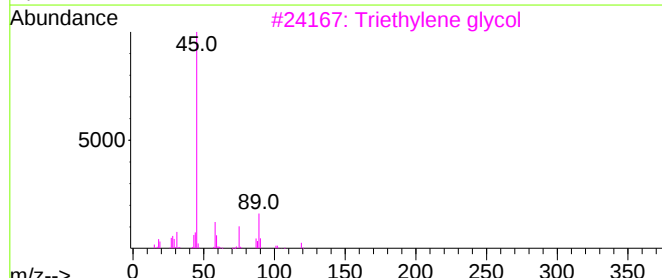
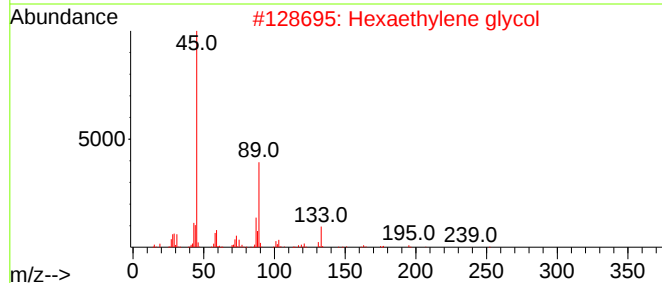
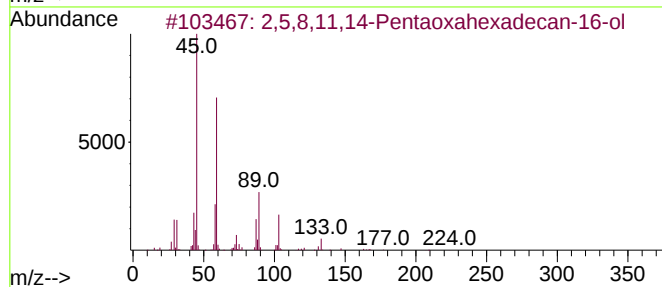
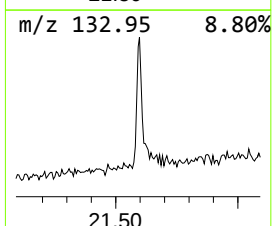
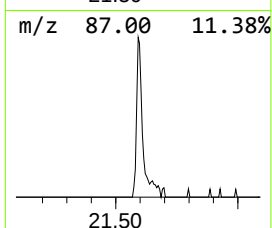
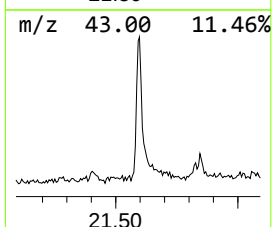
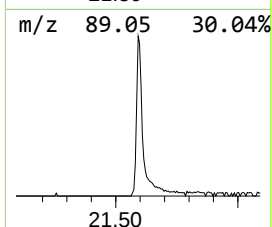
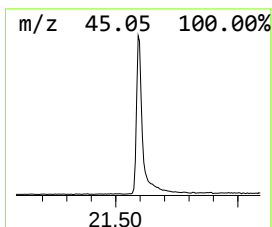
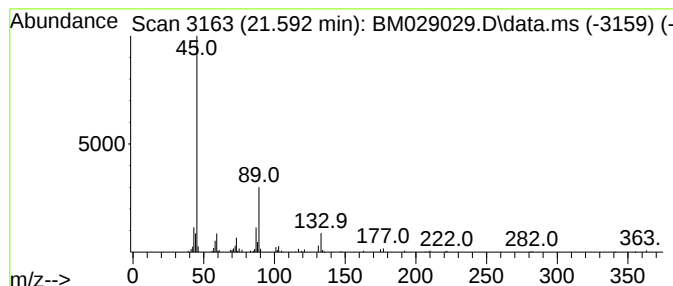
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,5,8,11,14-Pentaoxahexadec... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.592	17.77 ng	115100	Chrysene-d12	21.256

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6		023778-52-1	86
2	Hexaethylene glycol	282	C12H26O7		002615-15-8	78
3	Triethylene glycol	150	C6H14O4		000112-27-6	78
4	Pentaethylene glycol	238	C10H22O6		004792-15-8	78
5	Tetraethylene glycol	194	C8H18O5		000112-60-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029029.D
Acq On : 08 Mar 2021 21:21
Operator : CG/JU
Sample : M1582-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VEOLIA-72-11991

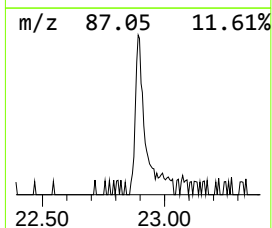
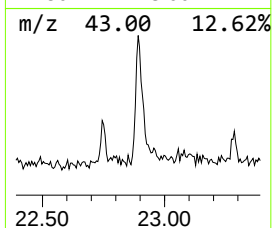
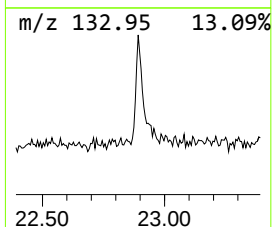
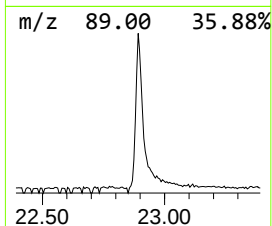
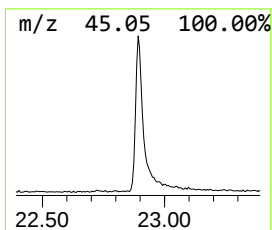
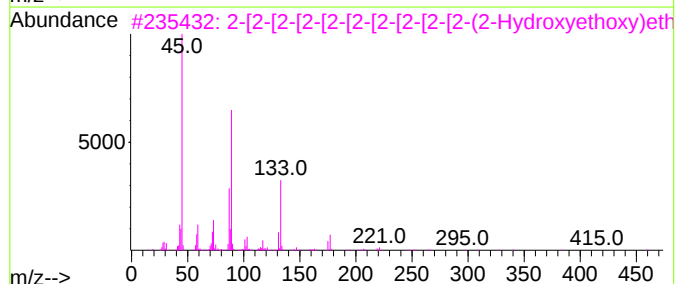
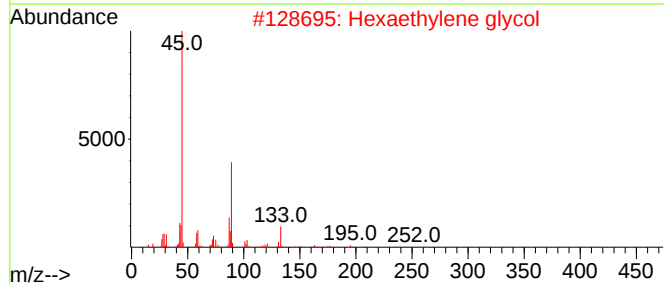
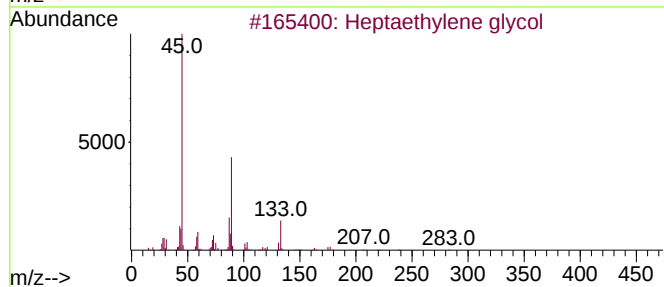
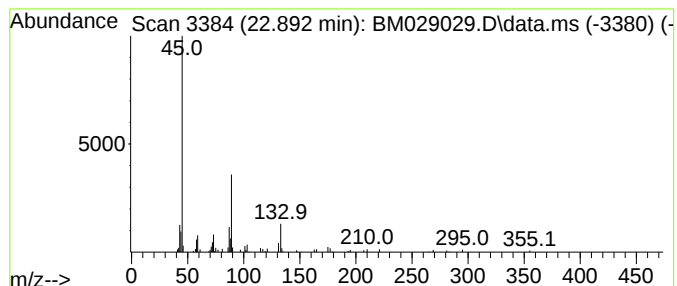
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptaethylene glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.892	12.13 ng	76563	Perylene-d12	23.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptaethylene glycol	326	C14H30O8	005617-32-3	91
2			Hexaethylene glycol	282	C12H26O7	002615-15-8	91
3			2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	91
4			2-[2-[2-[2-[2-[2-[2-[2-(2-...	546	C24H50O13	1000352-12-7	90
5			2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029029.D
Acq On : 08 Mar 2021 21:21
Operator : CG/JU
Sample : M1582-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VEOLIA-72-11991

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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
Isopropyl Alcohol	3.363	28.9	ng	83394	1	7.669	57795	20.0
unknown13.286	13.286	4.3	ng	20079	3	14.339	92791	20.0
unknown14.222	14.222	2.1	ng	9793	3	14.339	92791	20.0
n-Hexadecanoic ...	17.980	5.5	ng	28666	4	17.080	104109	20.0
Pentaethylene g...	18.751	4.7	ng	24426	4	17.080	104109	20.0
Tridecanoic acid	19.262	2.2	ng	14077	5	21.256	129562	20.0
Hexaethylene gl...	20.321	9.6	ng	62063	5	21.256	129562	20.0
Octadecyl trifl...	20.974	6.7	ng	43101	5	21.256	129562	20.0
2,5,8,11,14-Pen...	21.592	17.8	ng	115100	5	21.256	129562	20.0
Heptaethylene g...	22.892	12.1	ng	76563	6	23.415	126188	20.0