

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG121522\  
 Data File : BG055980.D  
 Acq On : 15 Dec 2022 17:07  
 Operator : CG/JU  
 Sample : N6048-01  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 MH-22

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-BG121322.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055980.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.407	14	20	25	rBV	15162	22143	2.97%	0.757%
2	5.416	357	362	368	rBB2	15344	21618	2.90%	0.739%
3	5.892	436	443	450	rBB	102288	162129	21.76%	5.540%
4	7.502	710	717	724	rBB	113756	189307	25.41%	6.469%
5	8.371	860	865	871	rBB	25617	42517	5.71%	1.453%
6	9.546	1058	1065	1072	rBB	65579	113242	15.20%	3.870%
7	11.203	1341	1347	1354	rBB	34294	61847	8.30%	2.113%
8	13.612	1750	1757	1763	rBB	252087	381374	51.19%	13.032%
9	14.981	1983	1990	1996	rBB	72244	110540	14.84%	3.777%
10	16.315	2212	2217	2223	rBB	19690	28147	3.78%	0.962%
11	16.456	2234	2241	2250	rBV	287070	429461	57.64%	14.676%
12	17.713	2449	2455	2461	rBV	108986	159722	21.44%	5.458%
13	18.565	2596	2600	2609	rBV2	14826	20697	2.78%	0.707%
14	19.817	2807	2813	2818	rBV4	5723	9530	1.28%	0.326%
15	20.293	2888	2894	2899	rBV	574718	745045	100.00%	25.460%
16	21.615	3114	3119	3124	rVB4	17103	26756	3.59%	0.914%
17	22.020	3181	3188	3195	rBV	111282	194996	26.17%	6.663%
18	25.522	3774	3784	3798	rVB2	67200	207296	27.82%	7.084%

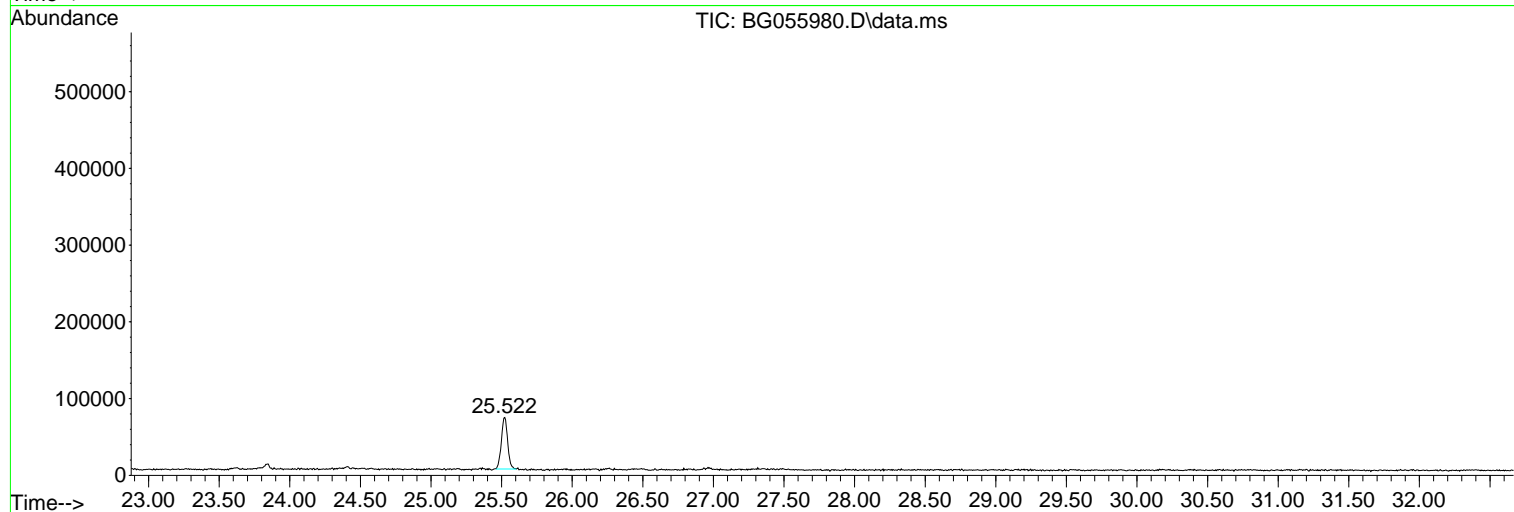
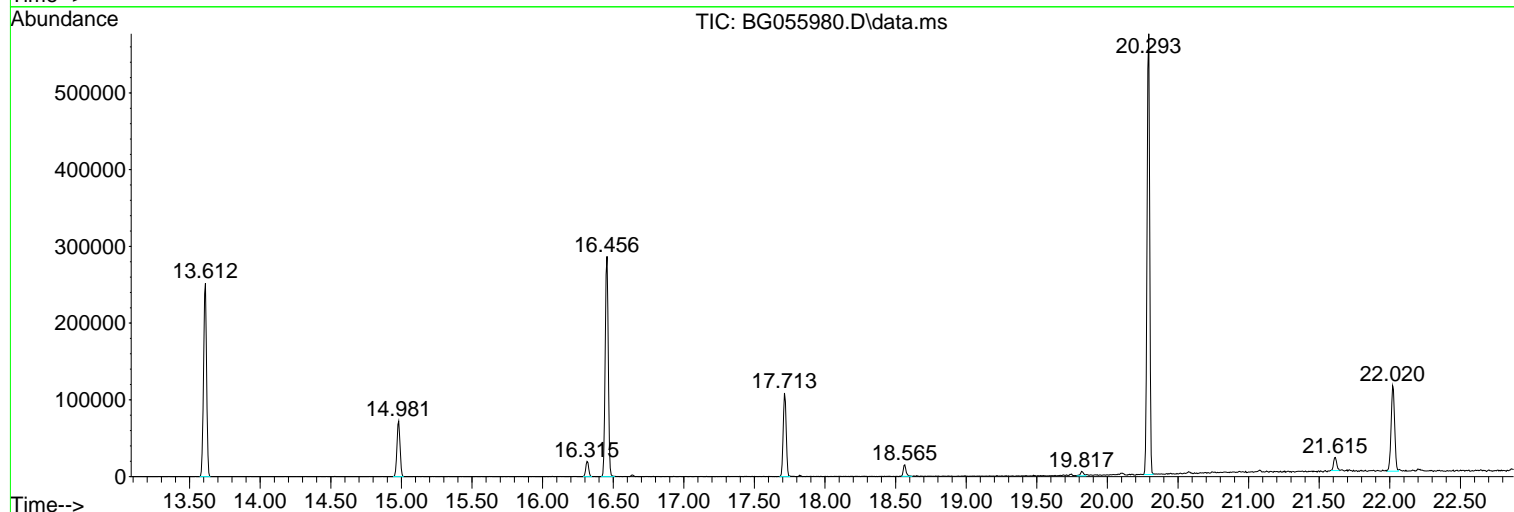
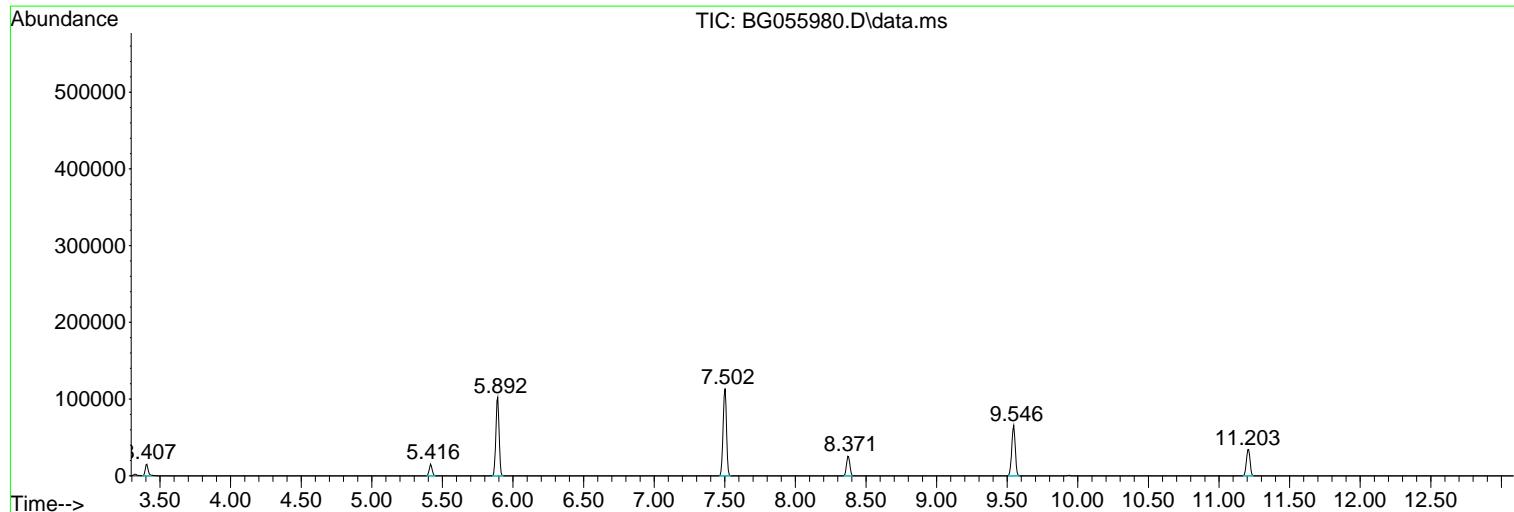
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG121322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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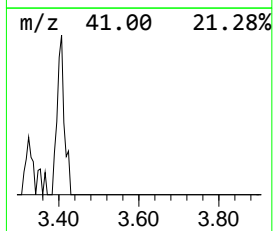
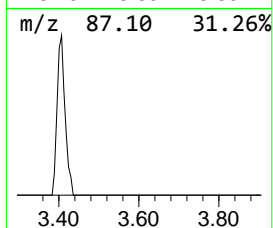
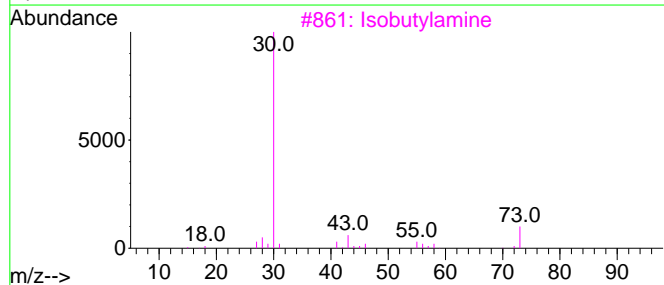
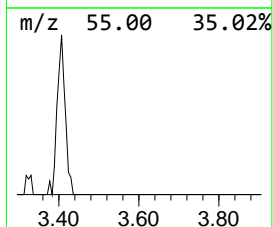
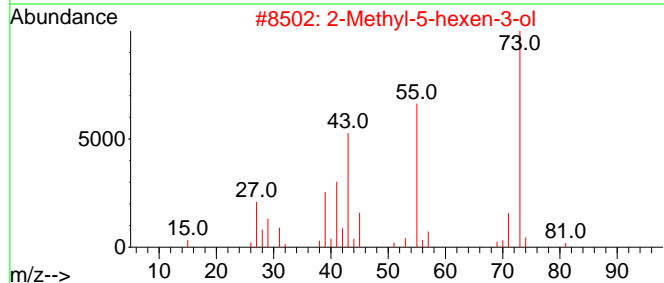
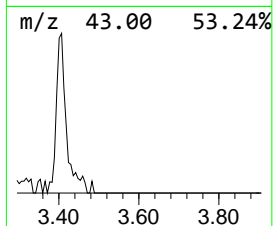
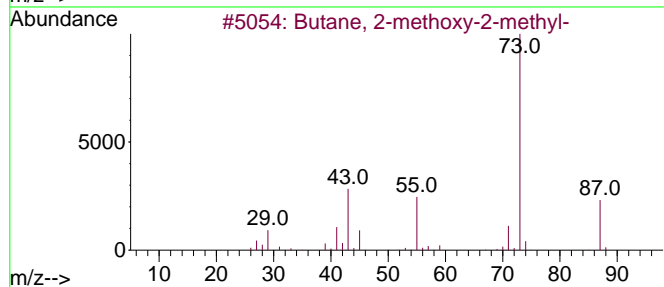
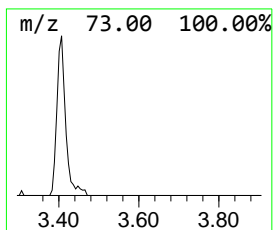
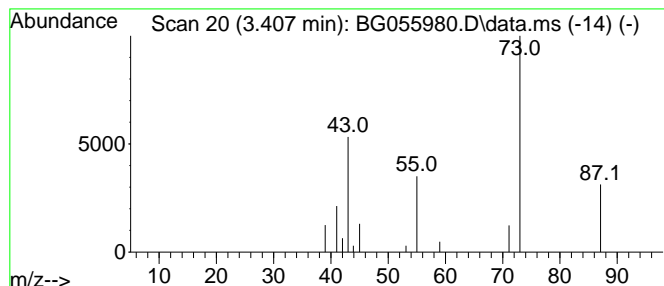
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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 Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.407	10.42 ng	22143	1,4-Dichlorobenzene-d4	8.377

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
3		Isobutylamine	73	C4H11N	000078-81-9	5
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5
5		(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	4



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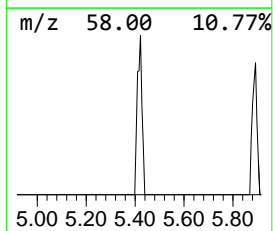
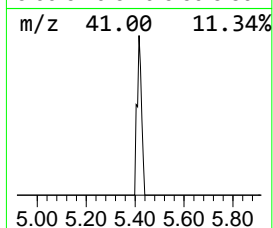
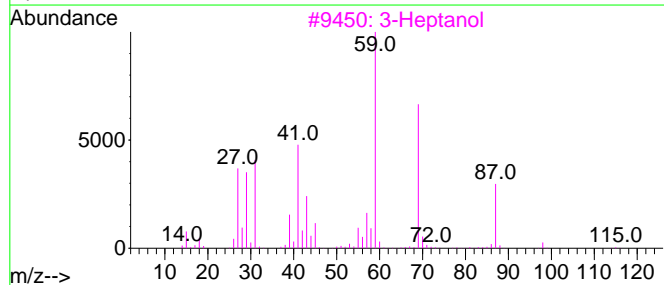
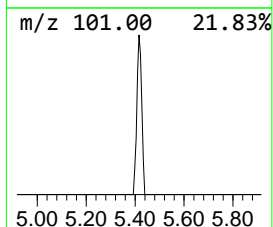
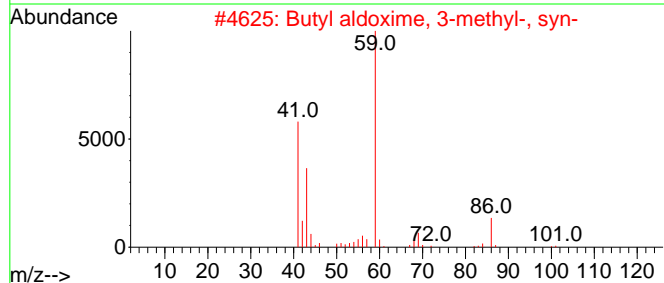
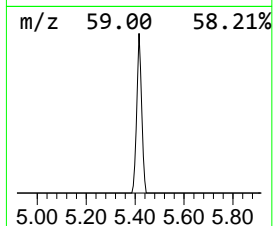
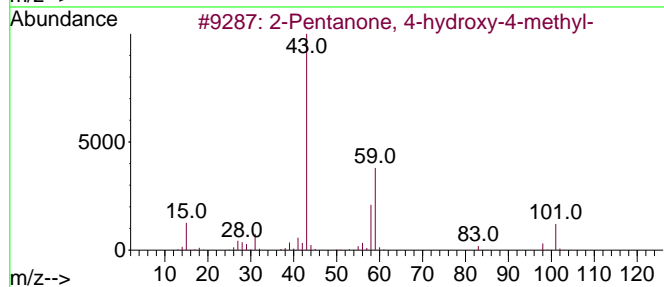
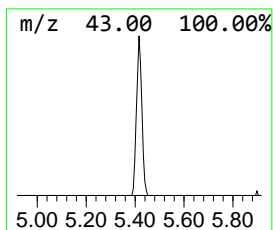
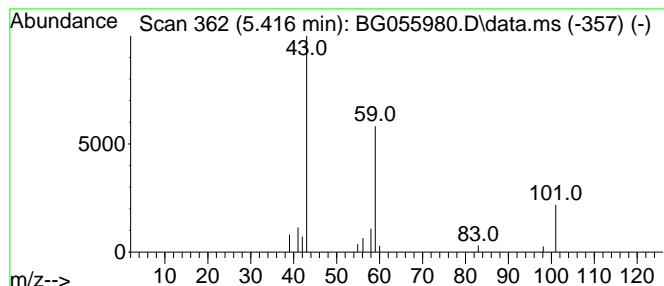
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.416	10.17 ng	21618	1,4-Dichlorobenzene-d4	8.377

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
3		3-Heptanol	116	C7H16O	000589-82-2	9
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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Instrument :  
 BNA\_G  
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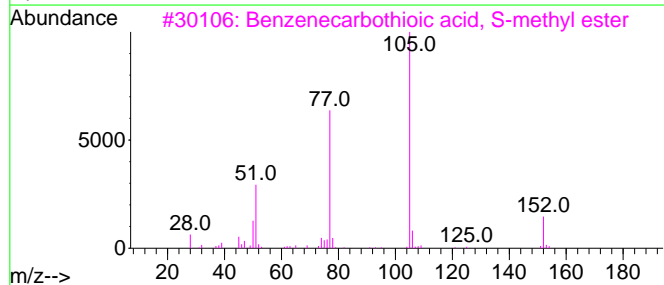
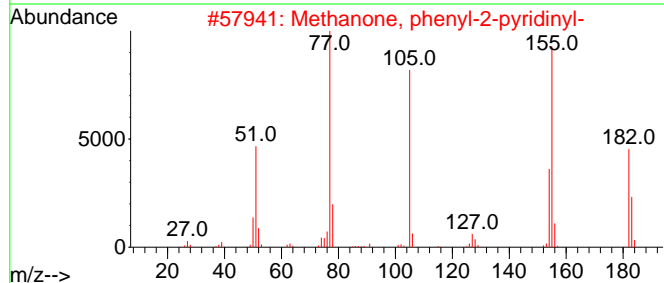
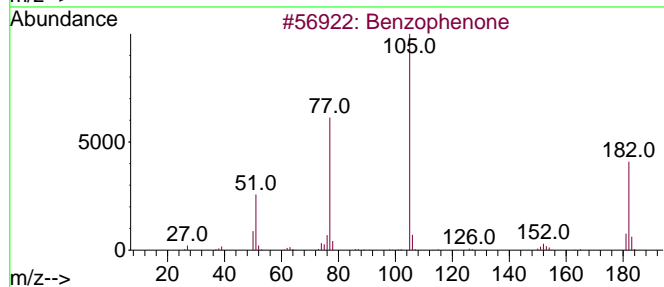
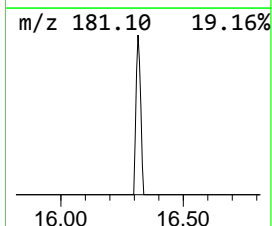
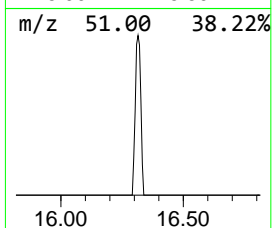
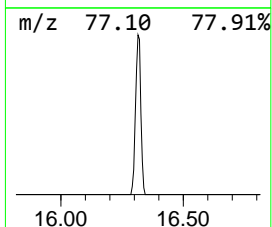
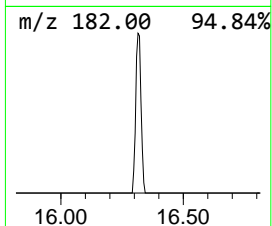
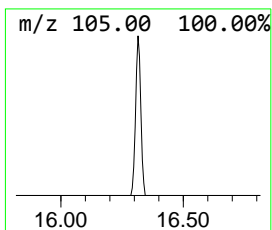
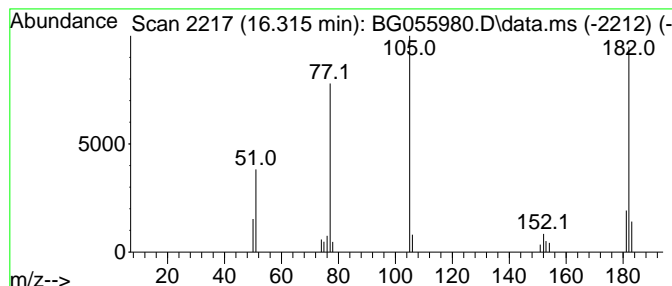
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG121322.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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 Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.315	5.09 ng	28147	Acenaphthene-d10	14.981

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	47
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	45
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	38
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	38



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 Sample : N6048-01  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_G  
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 MH-22

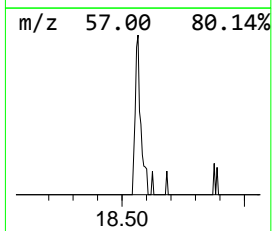
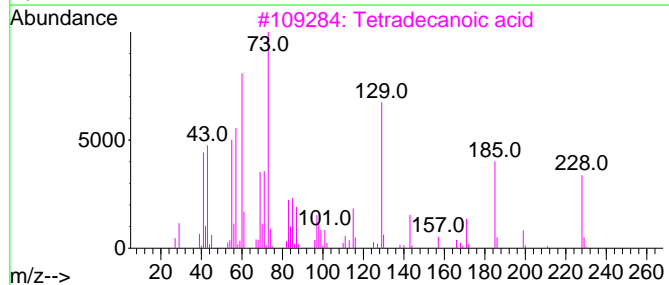
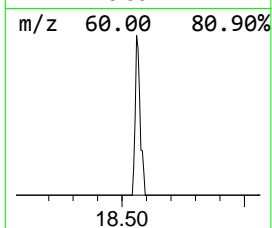
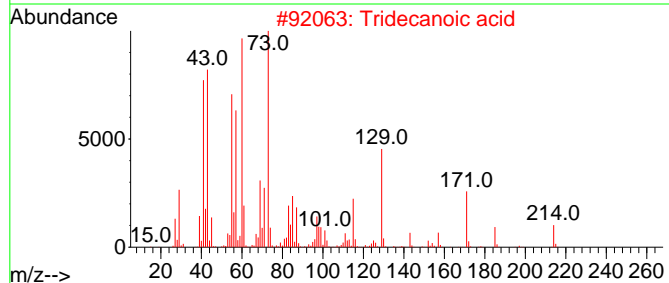
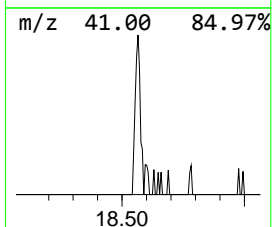
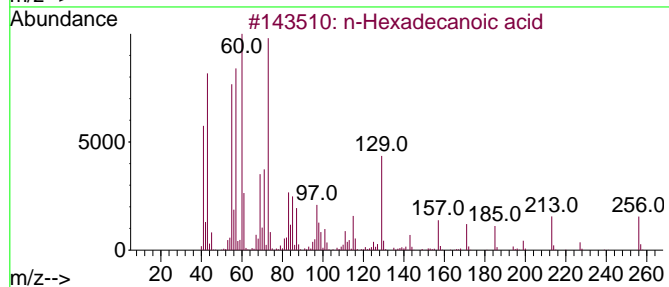
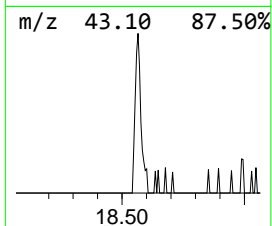
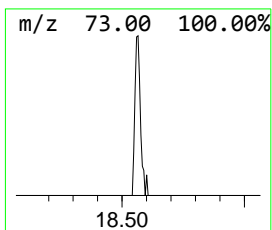
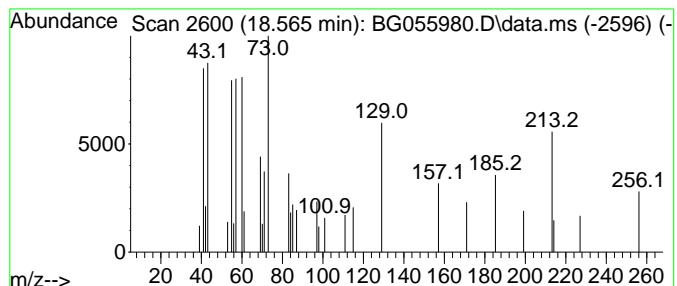
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG121322.M  
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TIC Library : C:\Database\NIST20.L  
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 Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.565	2.59 ng	20697	Phenanthrene-d10	17.713

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	45
5		Dodecanoic acid	200	C12H24O2	000143-07-7	38



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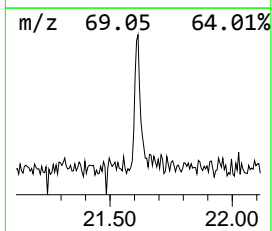
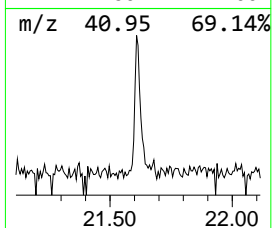
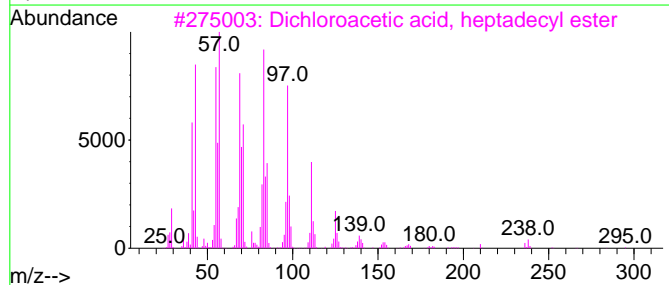
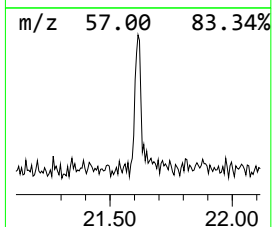
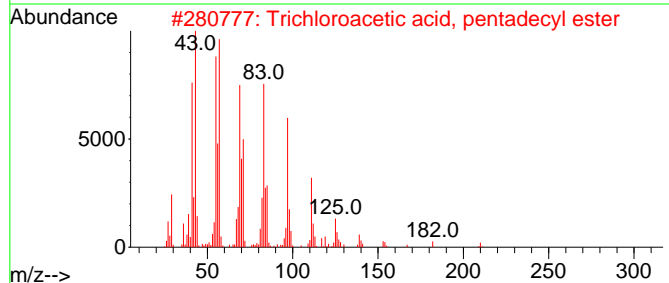
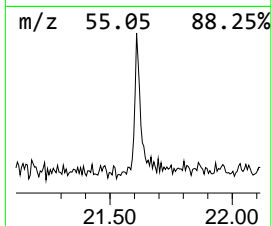
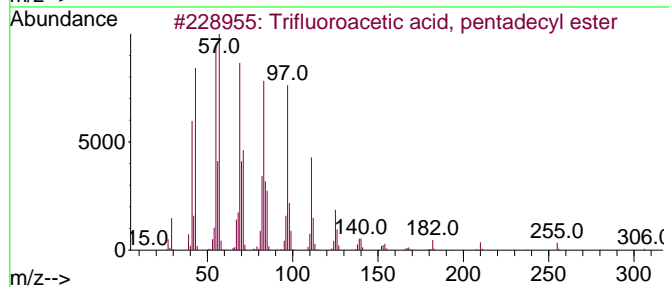
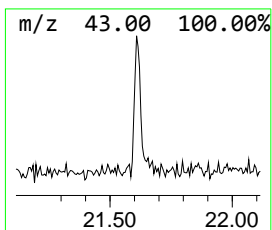
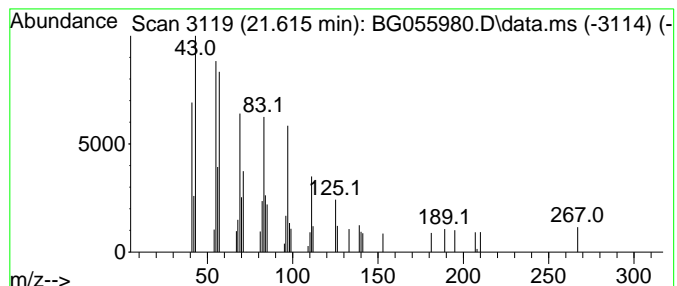
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG121322.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
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 Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.615	2.74 ng	26756	Chrysene-d12	22.020

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81
4		1-Docosene	308	C22H44	001599-67-3	81
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	81



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.407	10.4	ng	22143	1	8.377	42517	20.0
2-Pentanone, 4-...	5.416	10.2	ng	21618	1	8.377	42517	20.0
Benzophenone	16.315	5.1	ng	28147	3	14.981	110540	20.0
n-Hexadecanoic ...	18.565	2.6	ng	20697	4	17.713	159722	20.0
Trifluoroacetic...	21.615	2.7	ng	26756	5	22.020	194996	20.0