

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
 Data File : BG057065.D
 Acq On : 12 Apr 2023 15:41
 Operator : CG/JU
 Sample : 02292-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 IDW-SO-VB3-041123

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-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057065.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.435	318	323	330	rBV	33270	53336	4.84%	1.070%
2	5.923	399	406	416	rBV	285296	478609	43.42%	9.600%
3	7.538	673	681	689	rBV	292672	509446	46.22%	10.219%
4	8.408	822	829	836	rBV	57672	92464	8.39%	1.855%
5	9.582	1021	1029	1038	rBV	168639	304917	27.66%	6.116%
6	11.245	1305	1312	1319	rBV	66724	120996	10.98%	2.427%
7	13.648	1713	1721	1727	rBV	462333	708461	64.27%	14.210%
8	15.016	1947	1954	1961	rBV	104575	167367	15.18%	3.357%
9	16.356	2176	2182	2187	rVB	23927	34008	3.09%	0.682%
10	16.497	2200	2206	2215	rVB	380878	569645	51.68%	11.426%
11	17.760	2414	2421	2427	rBV	143054	213988	19.41%	4.292%
12	18.594	2557	2563	2574	rBV	54680	78815	7.15%	1.581%
13	19.845	2772	2776	2780	rBV4	18429	23600	2.14%	0.473%
14	20.327	2852	2858	2863	rBV	869691	1102263	100.00%	22.109%
15	21.637	3077	3081	3088	rVB5	27441	43428	3.94%	0.871%
16	22.071	3149	3155	3163	rBV2	136065	237448	21.54%	4.763%
17	22.929	3298	3301	3306	rVB3	9191	12711	1.15%	0.255%
18	25.614	3747	3758	3768	rBV2	76459	234016	21.23%	4.694%

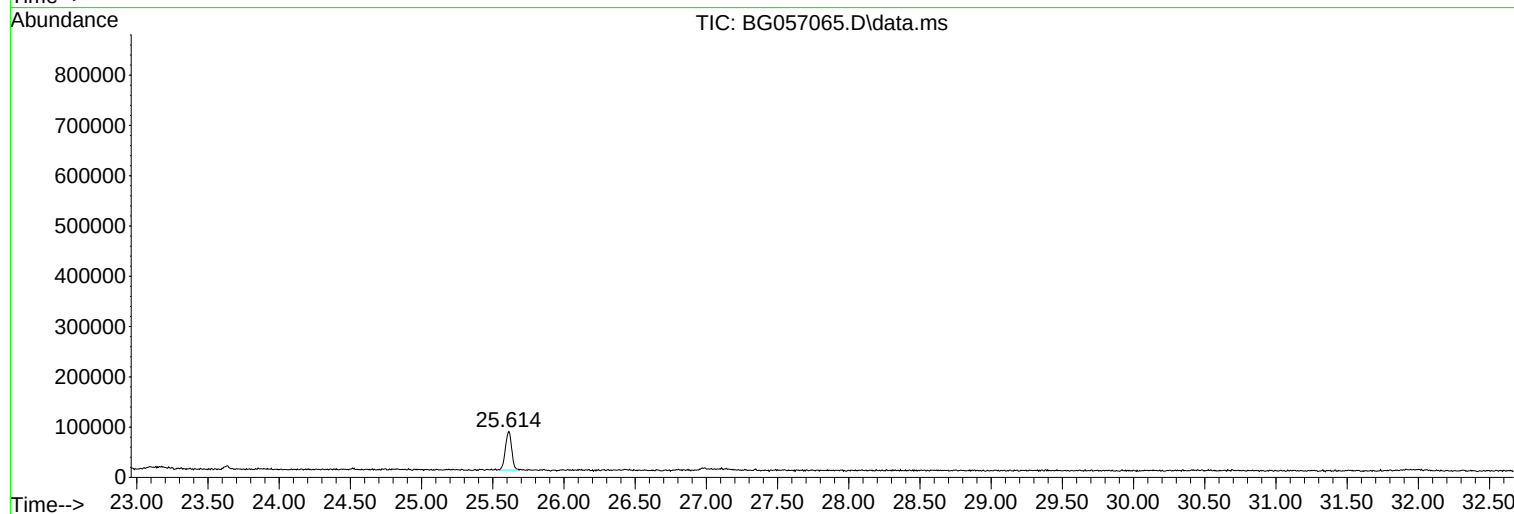
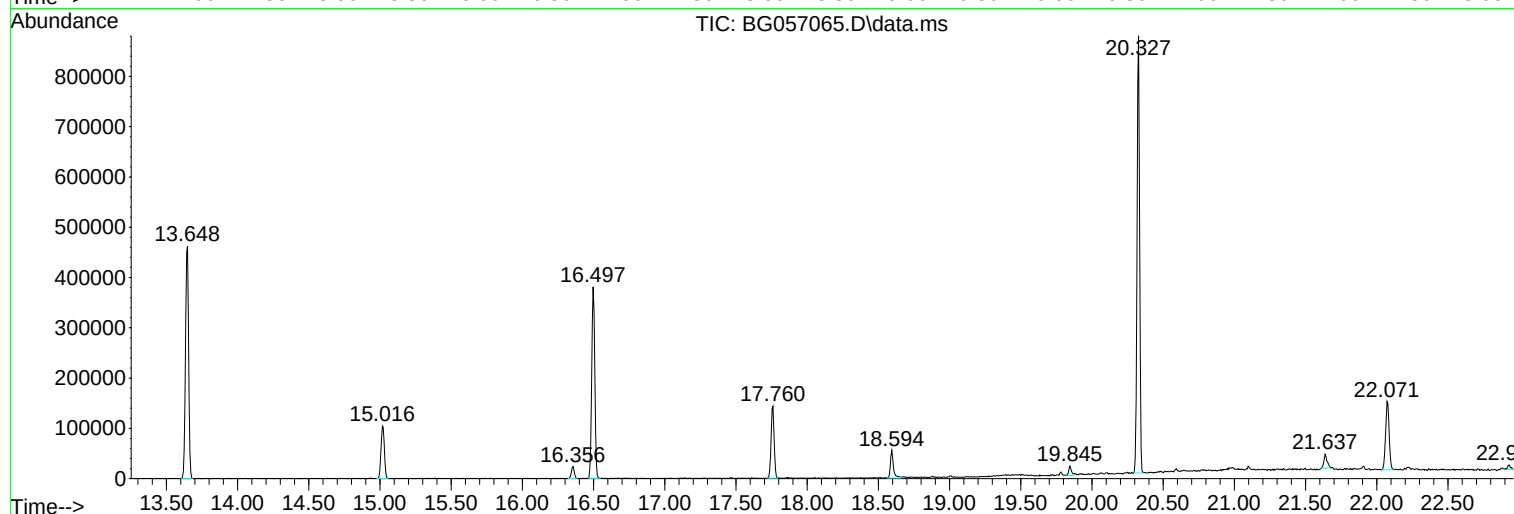
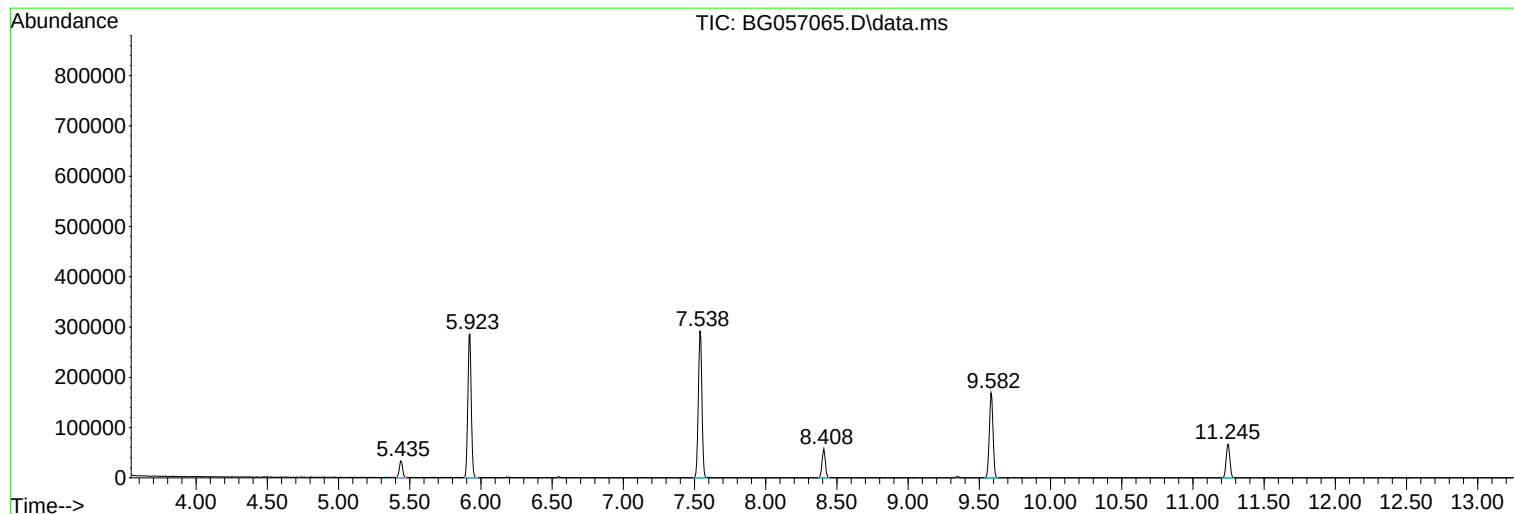
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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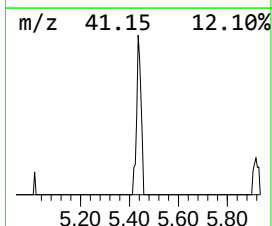
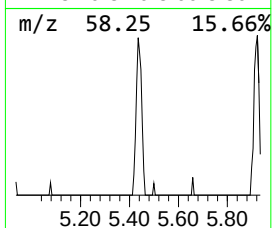
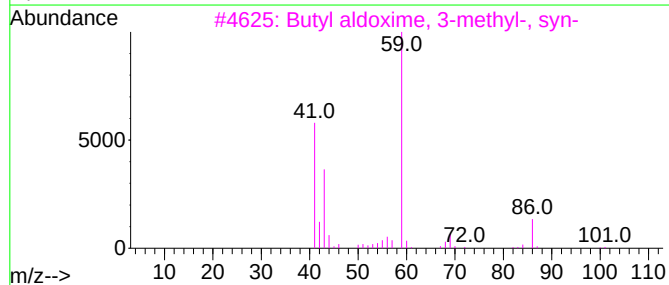
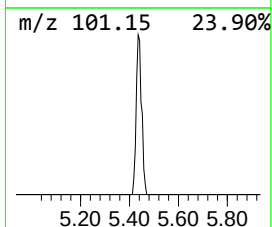
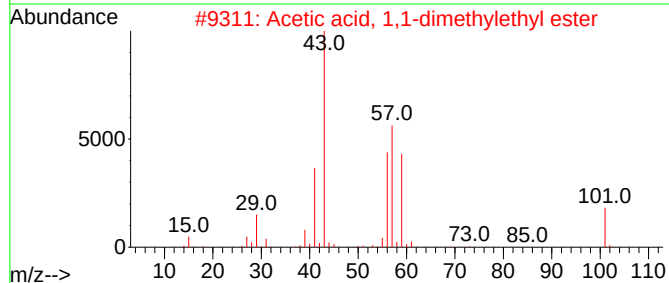
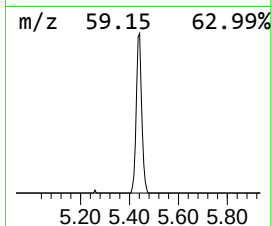
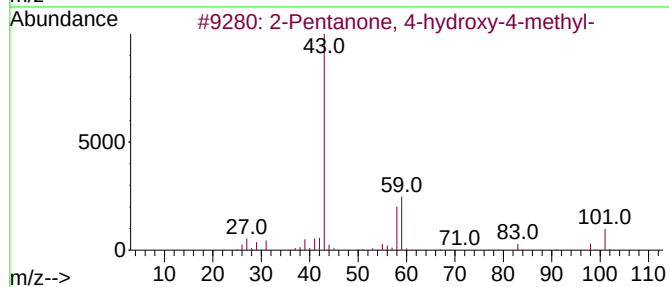
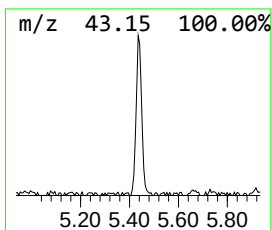
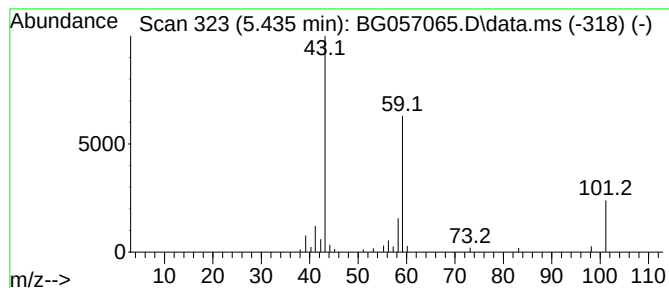
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.435	11.54 ng	53336	1,4-Dichlorobenzene-d4	8.408

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32		
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		



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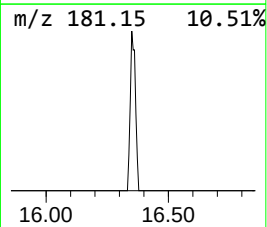
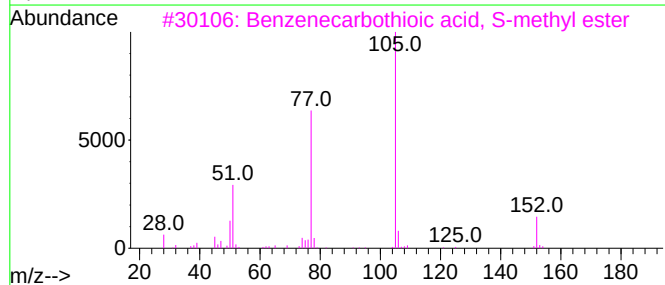
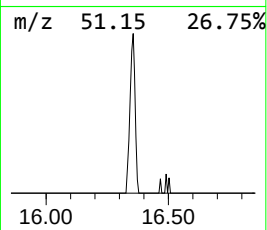
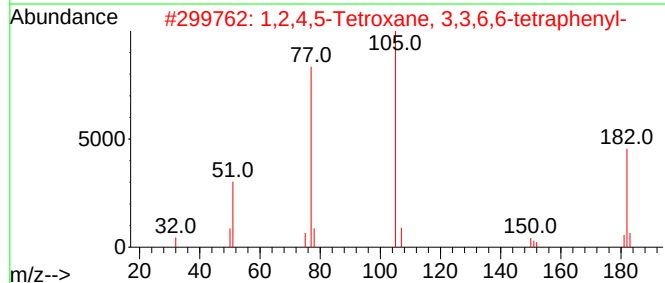
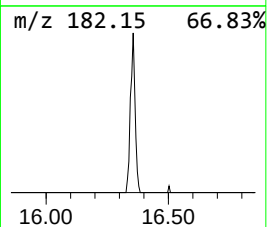
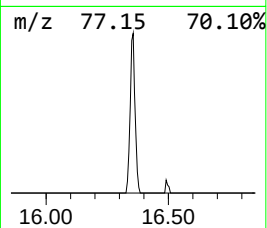
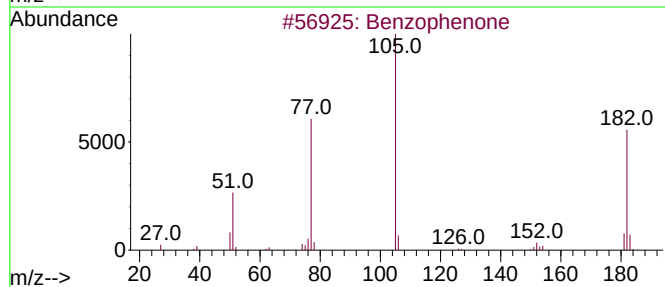
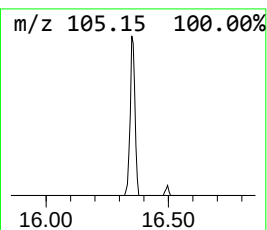
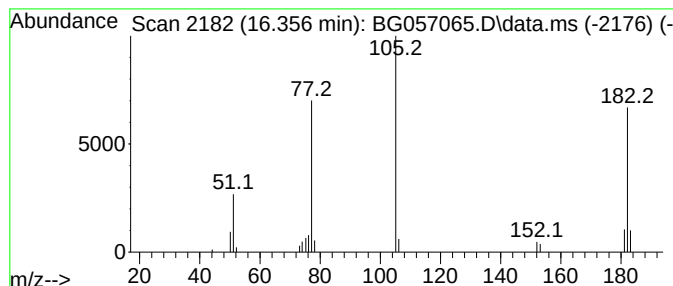
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.356	4.06 ng	34008	Acenaphthene-d10	15.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	91
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	43
4			Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	43
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	43



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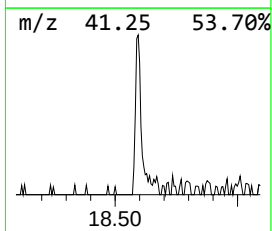
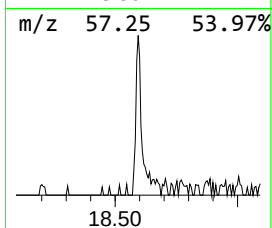
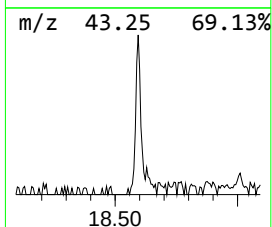
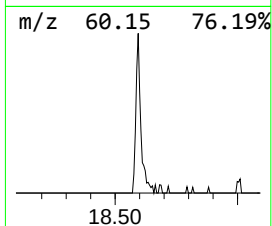
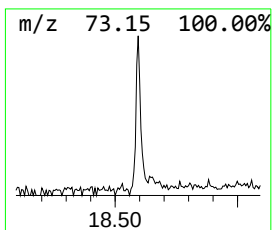
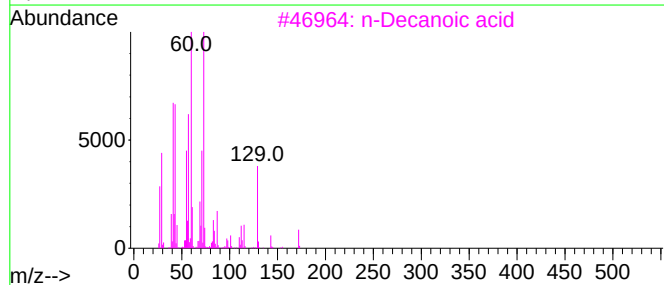
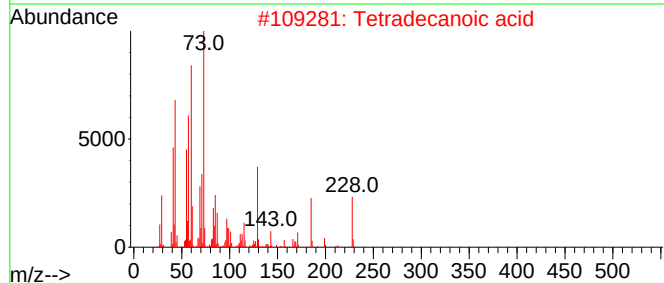
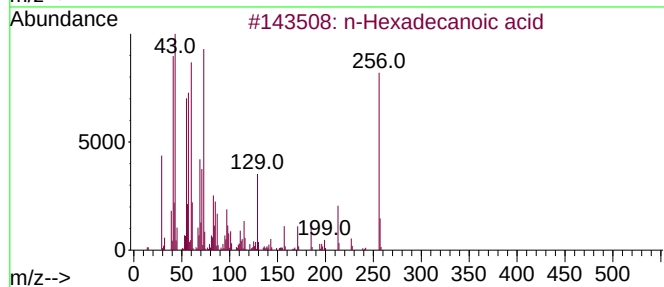
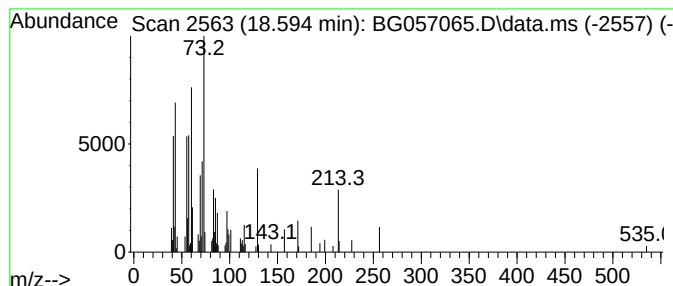
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.594	7.37 ng	78815	Phenanthrene-d10	17.760

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			n-Decanoic acid	172	C10H20O2	000334-48-5	76
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	68



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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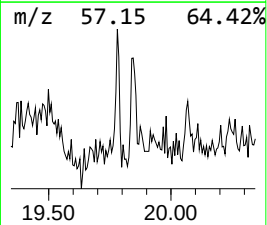
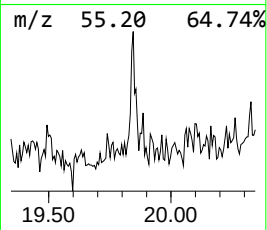
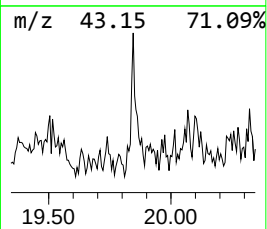
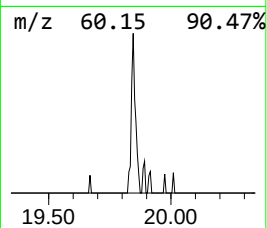
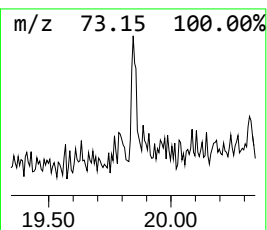
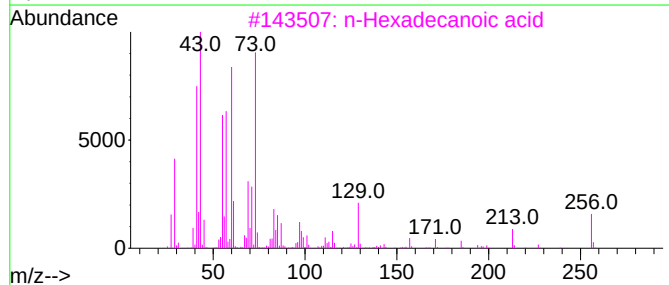
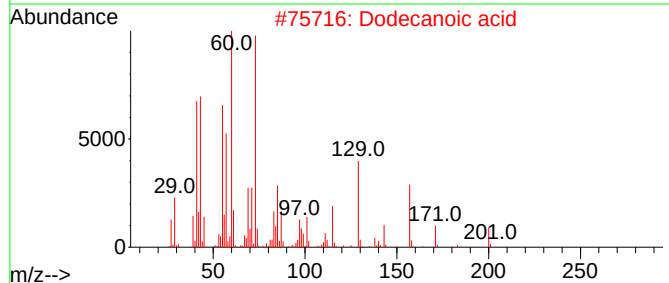
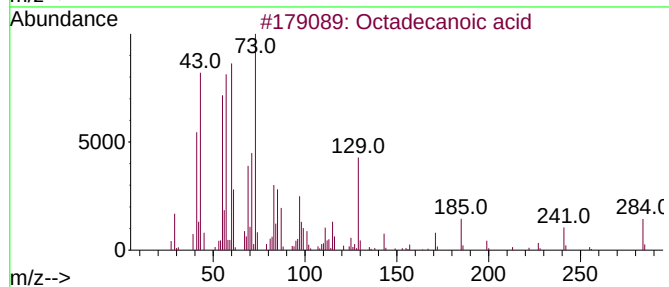
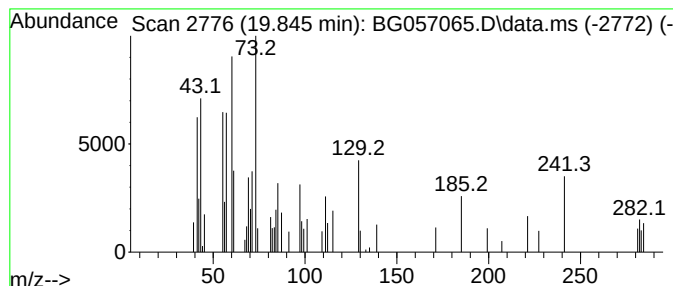
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.845	2.21 ng	23600	Phenanthrene-d10	17.760

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	89
2			Dodecanoic acid	200	C12H24O2	000143-07-7	49
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5			n-Decanoic acid	172	C10H20O2	000334-48-5	38



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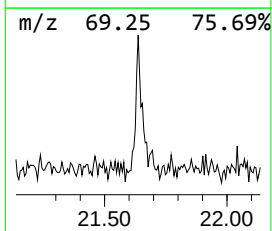
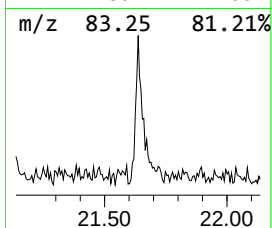
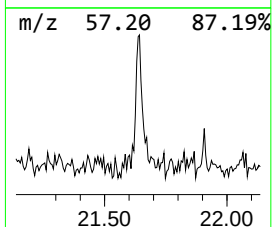
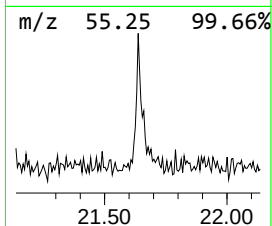
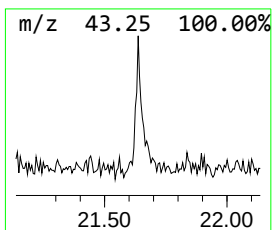
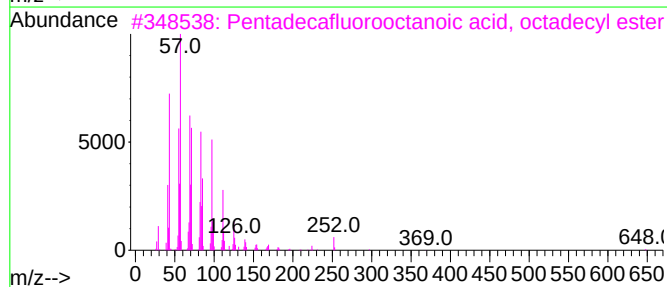
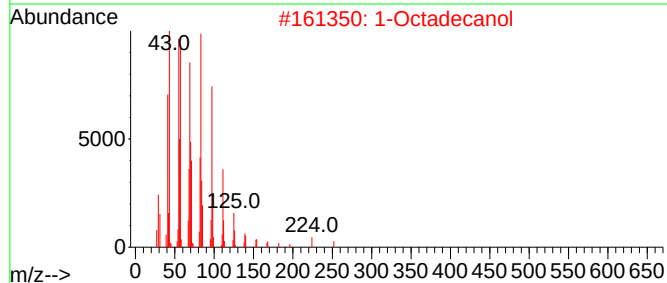
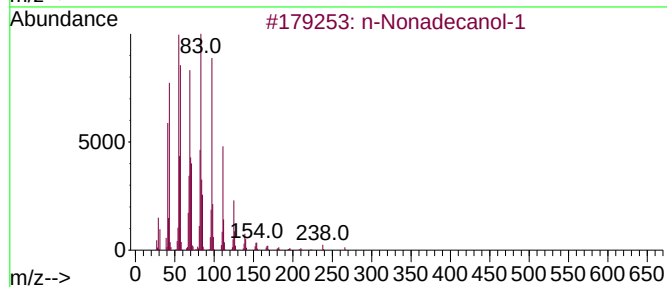
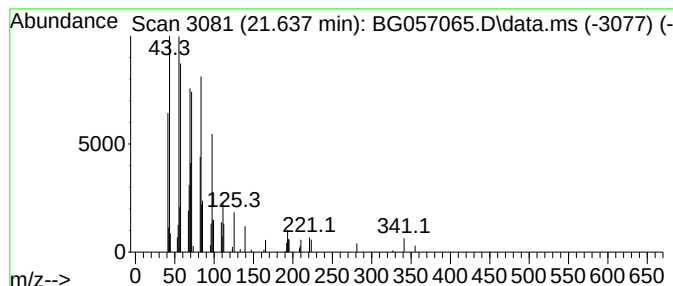
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.637	3.66 ng	43428	Chrysene-d12	22.077

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
2			1-Octadecanol	270	C18H38O	000112-92-5	81
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	80
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	76
5			Behenic alcohol	326	C22H46O	000661-19-8	74



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.435	11.5	ng	53336	1	8.408	92464	20.0
Benzophenone	16.356	4.1	ng	34008	3	15.016	167367	20.0
n-Hexadecanoic ...	18.594	7.4	ng	78815	4	17.760	213988	20.0
Octadecanoic acid	19.845	2.2	ng	23600	4	17.760	213988	20.0
n-Nonadecanol-1	21.637	3.7	ng	43428	5	22.077	237448	20.0