

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
 Data File : BG055745.D
 Acq On : 22 Nov 2022 18:36
 Operator : CG/JU
 Sample : N5749-08
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MH-83

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-BG111622.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055745.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.297	335	342	349	rVB	104714	162385	7.36%	1.356%
2	5.773	416	423	435	rBV	600328	959220	43.49%	8.008%
3	7.389	690	698	711	rBV	583593	1018387	46.17%	8.502%
4	8.240	837	843	852	rBV	129515	224922	10.20%	1.878%
5	9.416	1033	1043	1053	rBV	349920	630885	28.60%	5.267%
6	11.072	1316	1325	1332	rBV	174337	319622	14.49%	2.668%
7	13.493	1729	1737	1745	rBV	943766	1450205	65.75%	12.107%
8	14.862	1962	1970	1979	rVB	291413	465632	21.11%	3.887%
9	16.208	2190	2199	2206	rVB	48497	71244	3.23%	0.595%
10	16.349	2216	2223	2234	rBV	833814	1286636	58.34%	10.742%
11	17.606	2430	2437	2443	rBV	420347	608070	27.57%	5.077%
12	18.340	2558	2562	2571	rBV5	13808	29810	1.35%	0.249%
13	18.464	2578	2583	2600	rBV	245090	405132	18.37%	3.382%
14	18.881	2650	2654	2659	rVB2	26041	32170	1.46%	0.269%
15	19.610	2771	2778	2781	rBV7	16228	33196	1.51%	0.277%
16	19.639	2781	2783	2791	rVV2	15338	30015	1.36%	0.251%
17	19.727	2793	2798	2813	rBV3	56780	128780	5.84%	1.075%
18	20.191	2871	2877	2883	rBV	1654031	2205520	100.00%	18.413%
19	21.501	3096	3100	3113	rBV	107043	242914	11.01%	2.028%
20	21.901	3162	3168	3181	rVB2	414656	719686	32.63%	6.008%
21	23.646	3459	3465	3473	rVB	116897	232447	10.54%	1.941%
22	25.309	3739	3748	3761	rVB2	252762	721235	32.70%	6.021%

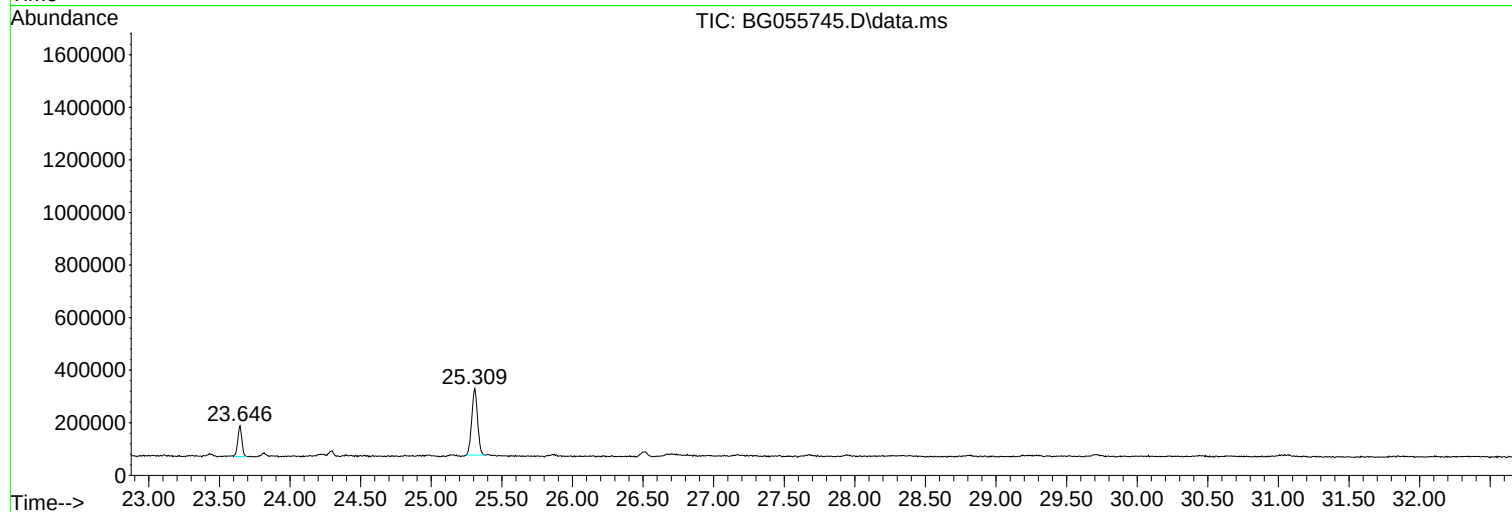
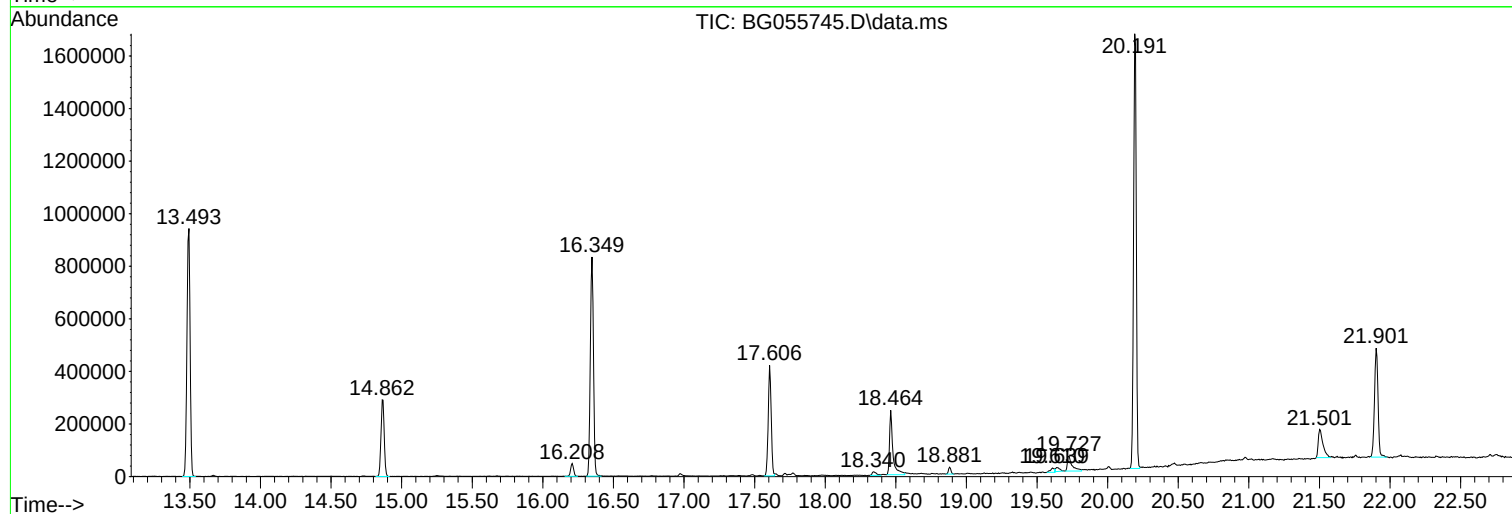
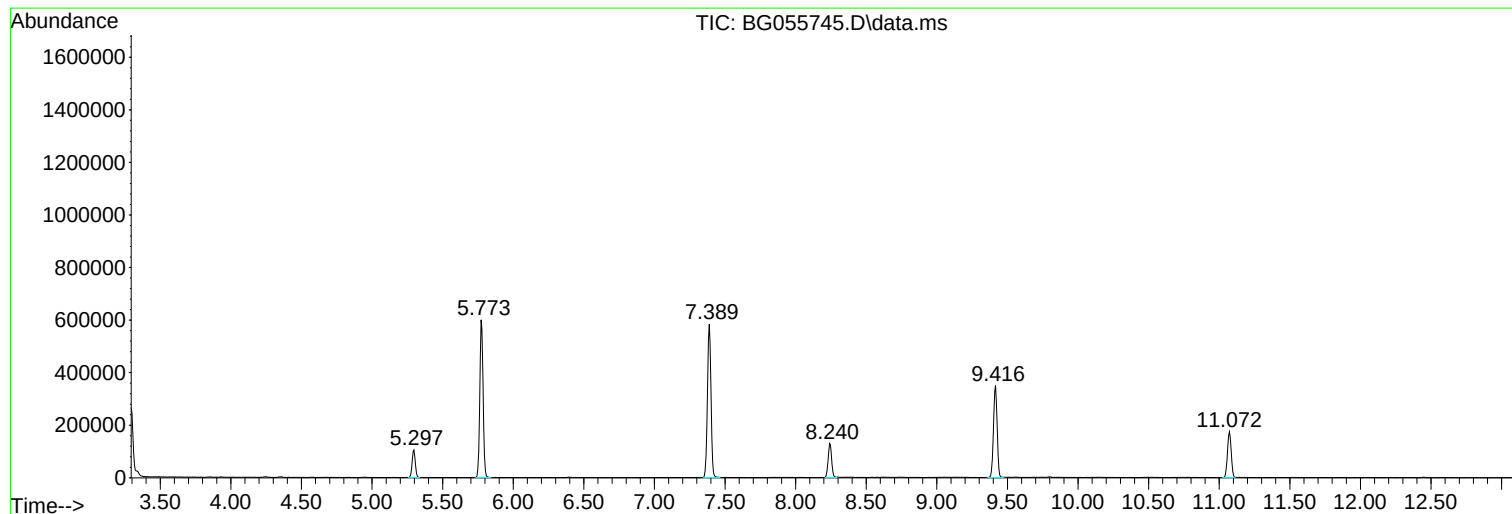
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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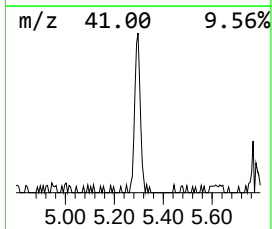
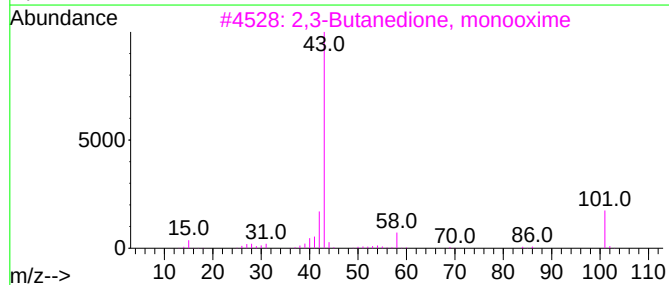
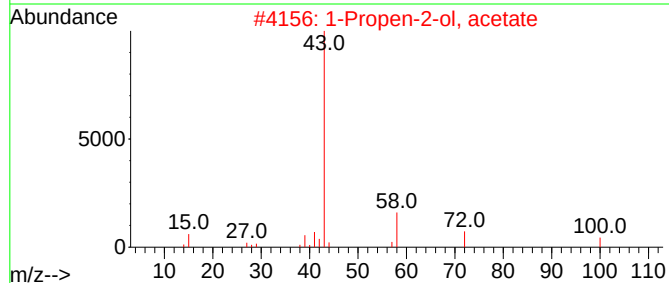
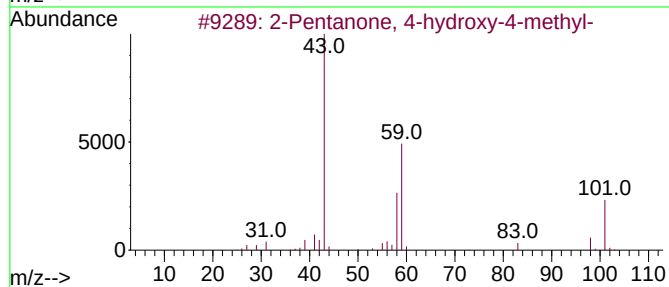
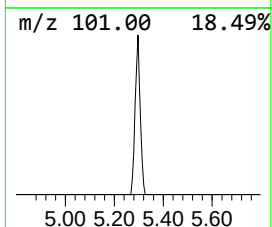
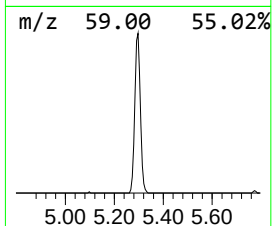
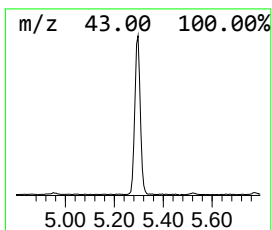
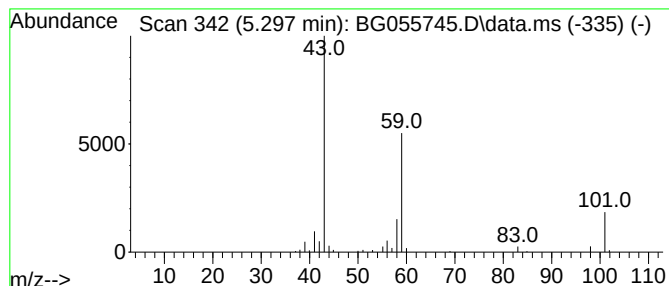
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.297	14.44 ng	162385	1,4-Dichlorobenzene-d4	8.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		



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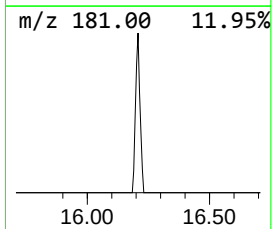
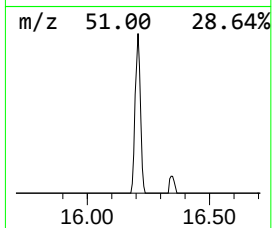
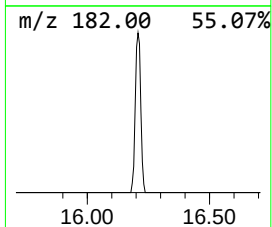
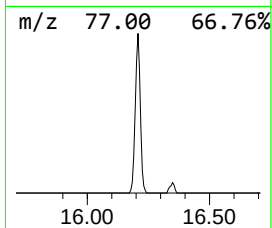
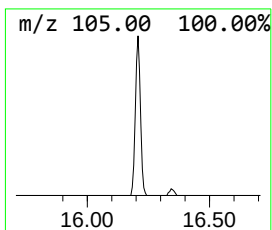
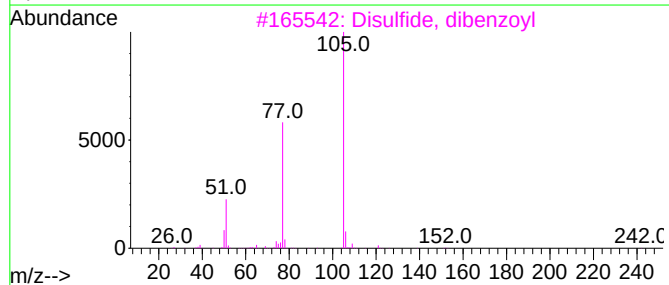
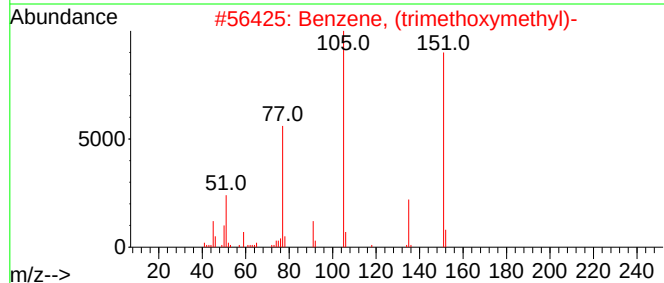
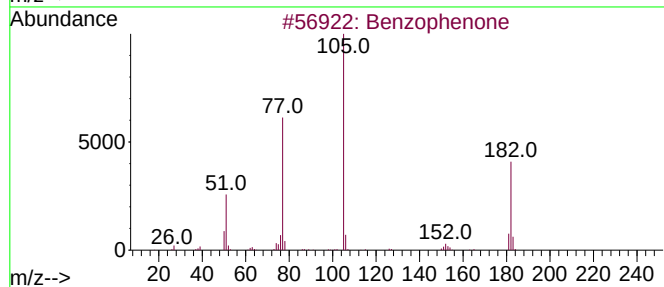
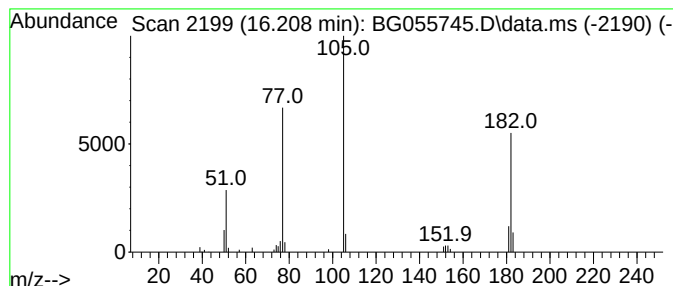
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Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.208	3.06 ng	71244	Acenaphthene-d10	14.862

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			Benzene, (trimethoxymethyl)-	182	C10H14O3	000707-07-3	47
3			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47
5			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47



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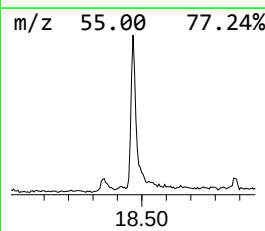
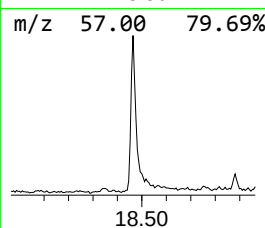
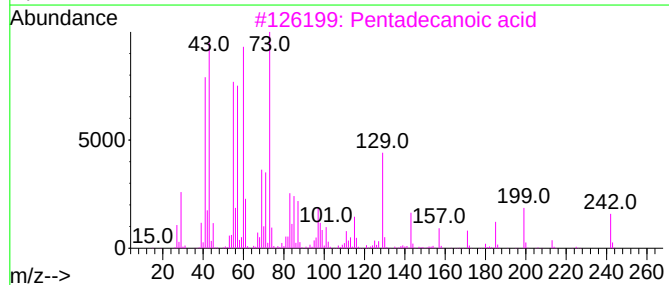
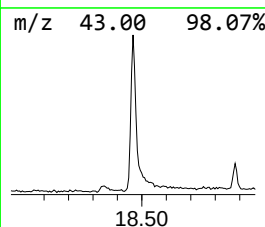
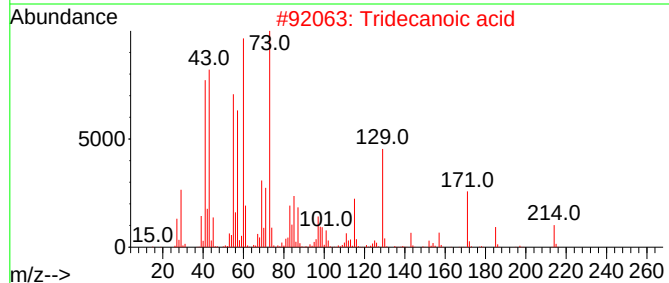
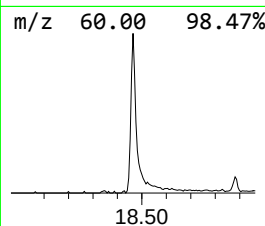
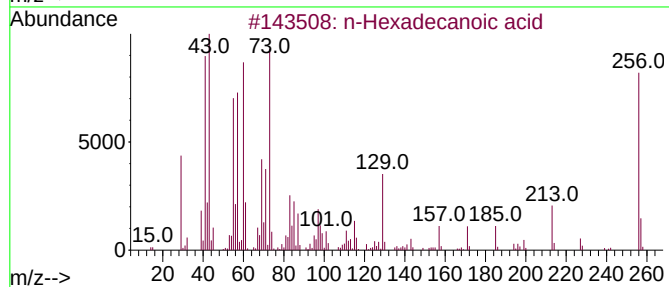
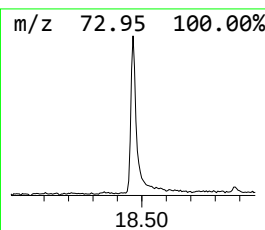
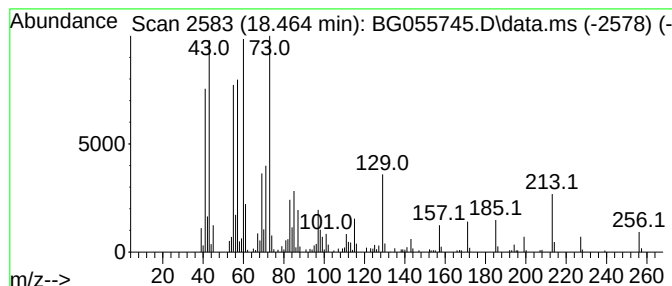
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.464	13.33 ng	405132	Phenanthrene-d10	17.606

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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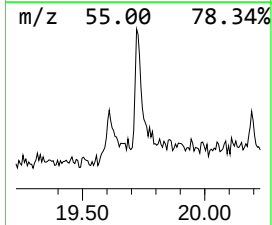
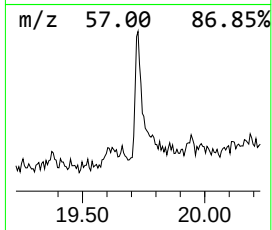
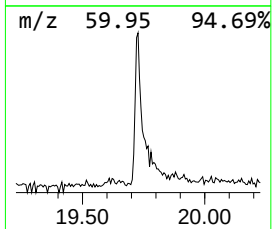
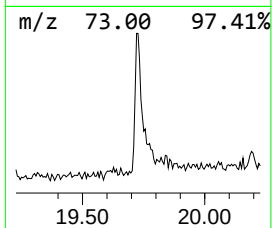
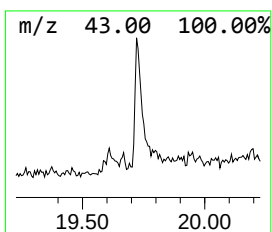
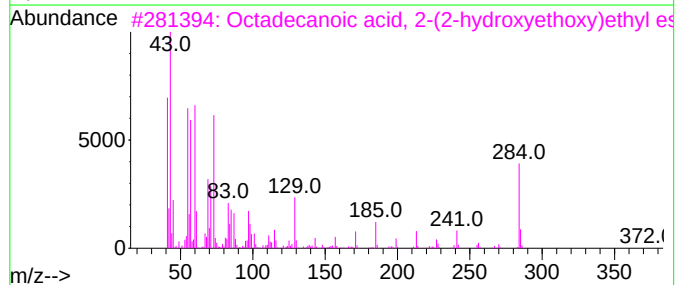
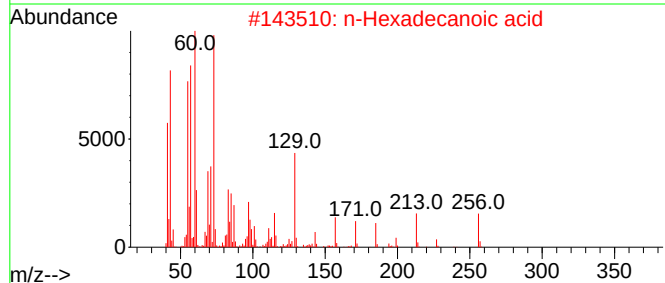
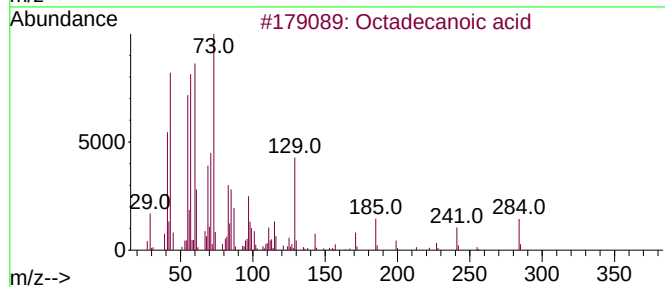
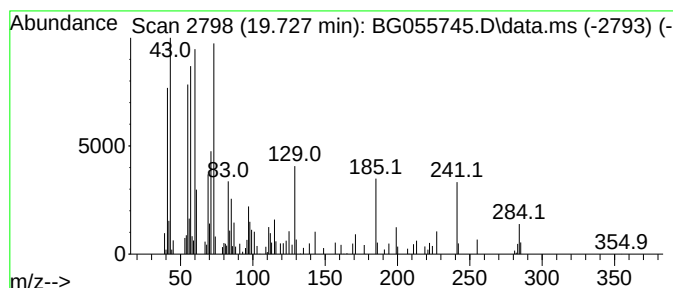
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.727	4.24 ng	128780	Phenanthrene-d10	17.606

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	78
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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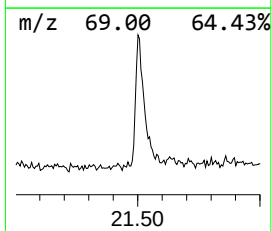
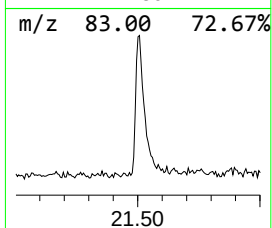
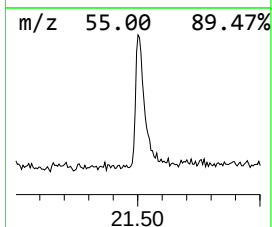
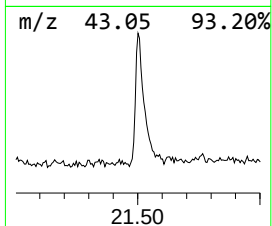
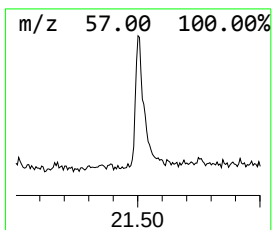
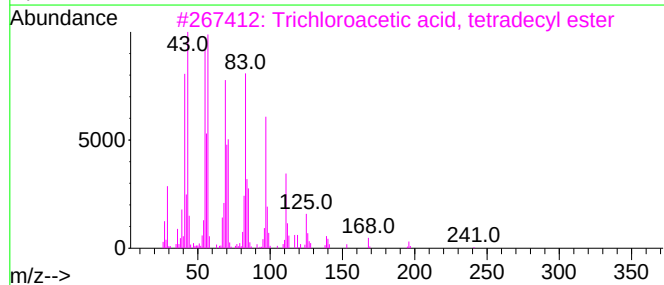
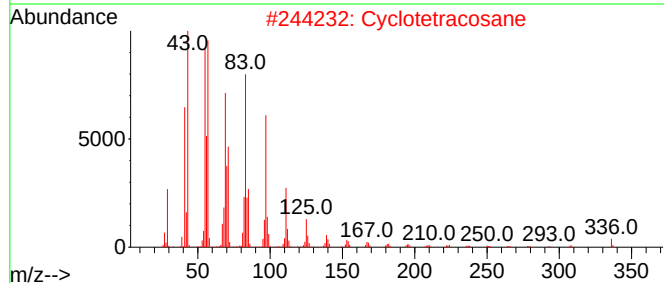
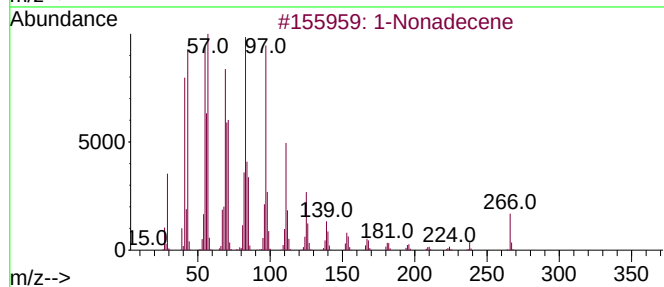
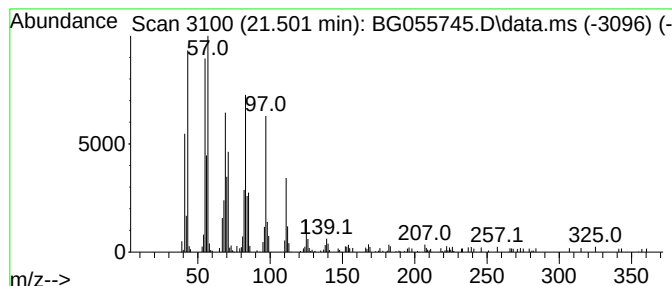
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Peak Number 5 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.501	6.75 ng	242914	Chrysene-d12	21.901

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	99
2	Cyclotetracosane			336	C24H48	000297-03-0	95
3	Trichloroacetic acid, tetradecyl...			358	C16H29Cl3O2	074339-52-9	95
4	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	94
5	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	94



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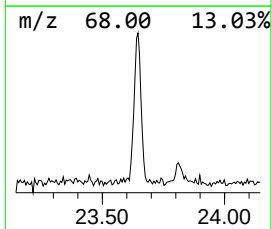
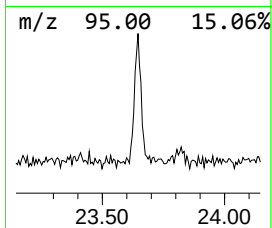
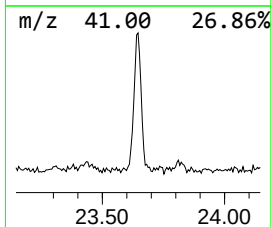
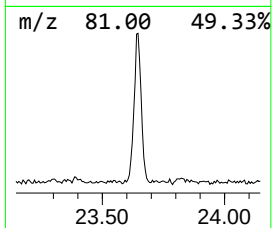
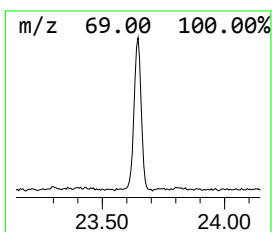
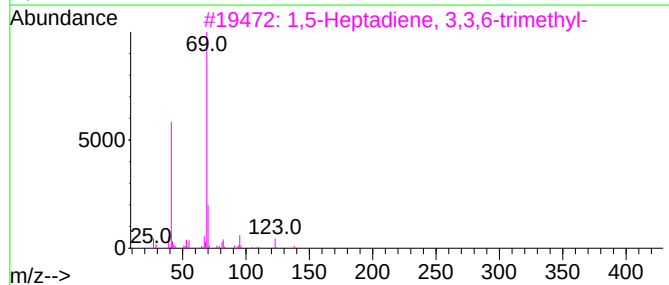
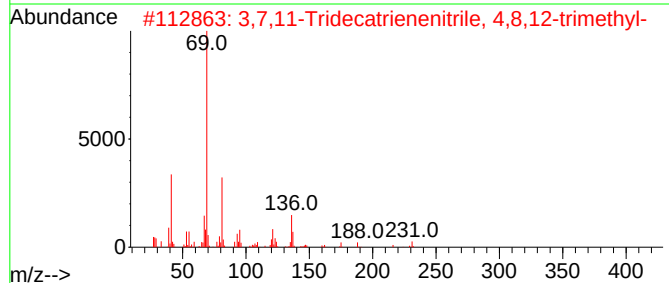
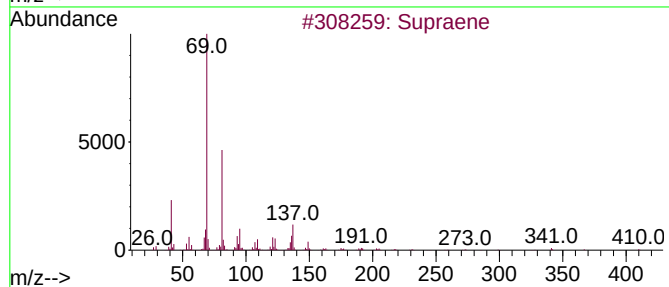
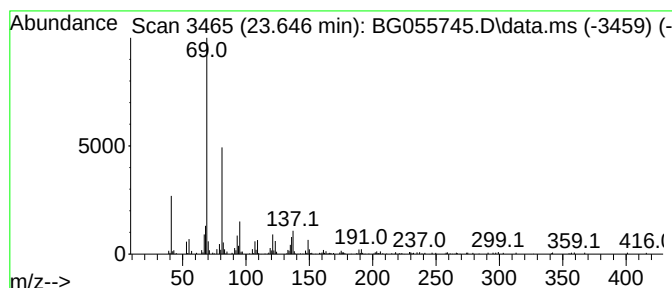
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.646	6.45 ng	232447	Perylene-d12	25.309

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Supraene	410	C30H50	007683-64-9	91
2		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72
3		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
4		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	52
5		1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
Data File : BG055745.D
Acq On : 22 Nov 2022 18:36
Operator : CG/JU
Sample : N5749-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-83

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.297	14.4	ng	162385	1	8.246	224922	20.0
Benzophenone	16.208	3.1	ng	71244	3	14.862	465632	20.0
n-Hexadecanoic ...	18.464	13.3	ng	405132	4	17.606	608070	20.0
Octadecanoic acid	19.727	4.2	ng	128780	4	17.606	608070	20.0
1-Nonadecene	21.501	6.8	ng	242914	5	21.901	719686	20.0
Supraene	23.646	6.5	ng	232447	6	25.309	721235	20.0