

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052523\
 Data File : BG057573.D
 Acq On : 26 May 2023 1:24
 Operator : CG/JU
 Sample : 02935-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ETGI-346

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-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057573.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	307	314	319	rBV	21109	32871	2.72%	0.423%
2	5.873	390	397	406	rBV	318701	522449	43.27%	6.717%
3	7.500	666	674	687	rBV	345806	606782	50.26%	7.801%
4	8.352	812	819	825	rBV	88659	149229	12.36%	1.919%
5	9.533	1011	1020	1032	rVB	208571	379092	31.40%	4.874%
6	11.189	1295	1302	1308	rBV	122325	219751	18.20%	2.825%
7	13.592	1702	1711	1718	rBV	604058	909433	75.32%	11.693%
8	14.967	1938	1945	1952	rVB	191674	308697	25.57%	3.969%
9	16.300	2167	2172	2180	rVB	86025	131293	10.87%	1.688%
10	16.453	2191	2198	2205	rBV	426247	673586	55.79%	8.660%
11	17.704	2405	2411	2415	rBV	242414	365904	30.31%	4.704%
12	17.751	2415	2419	2425	rVB	79391	121381	10.05%	1.561%
13	17.839	2430	2434	2442	rVB	14263	22209	1.84%	0.286%
14	18.109	2475	2480	2490	rBV7	7976	20950	1.74%	0.269%
15	18.538	2549	2553	2557	rBV	70923	99142	8.21%	1.275%
16	18.620	2563	2567	2573	rVB2	23255	34588	2.86%	0.445%
17	18.773	2586	2593	2596	rBV3	17745	37300	3.09%	0.480%
18	19.061	2638	2642	2645	rBV	10892	13688	1.13%	0.176%
19	19.114	2648	2651	2657	rVB5	13051	18130	1.50%	0.233%
20	19.472	2708	2712	2715	rBV2	11682	16062	1.33%	0.207%
21	19.619	2733	2737	2743	rBV3	14150	24661	2.04%	0.317%
22	19.742	2751	2758	2762	rVB	188123	271015	22.45%	3.484%
23	19.789	2762	2766	2771	rBV7	18017	31881	2.64%	0.410%
24	20.065	2808	2813	2815	rBV2	29967	50435	4.18%	0.648%
25	20.101	2815	2819	2824	rVV	170170	237981	19.71%	3.060%
26	20.159	2827	2829	2834	rVB4	11539	14538	1.20%	0.187%
27	20.277	2843	2849	2855	rBV	915660	1207362	100.00%	15.523%
28	21.375	3033	3036	3042	rVB2	23791	34167	2.83%	0.439%
29	21.563	3065	3068	3074	rBV2	53639	78102	6.47%	1.004%
30	22.010	3136	3144	3150	rBV2	228695	534921	44.30%	6.877%
31	22.063	3150	3153	3162	rVB	78454	131662	10.90%	1.693%
32	24.395	3544	3550	3557	rBV2	65945	184805	15.31%	2.376%
33	25.517	3734	3741	3750	rVB2	105658	293781	24.33%	3.777%

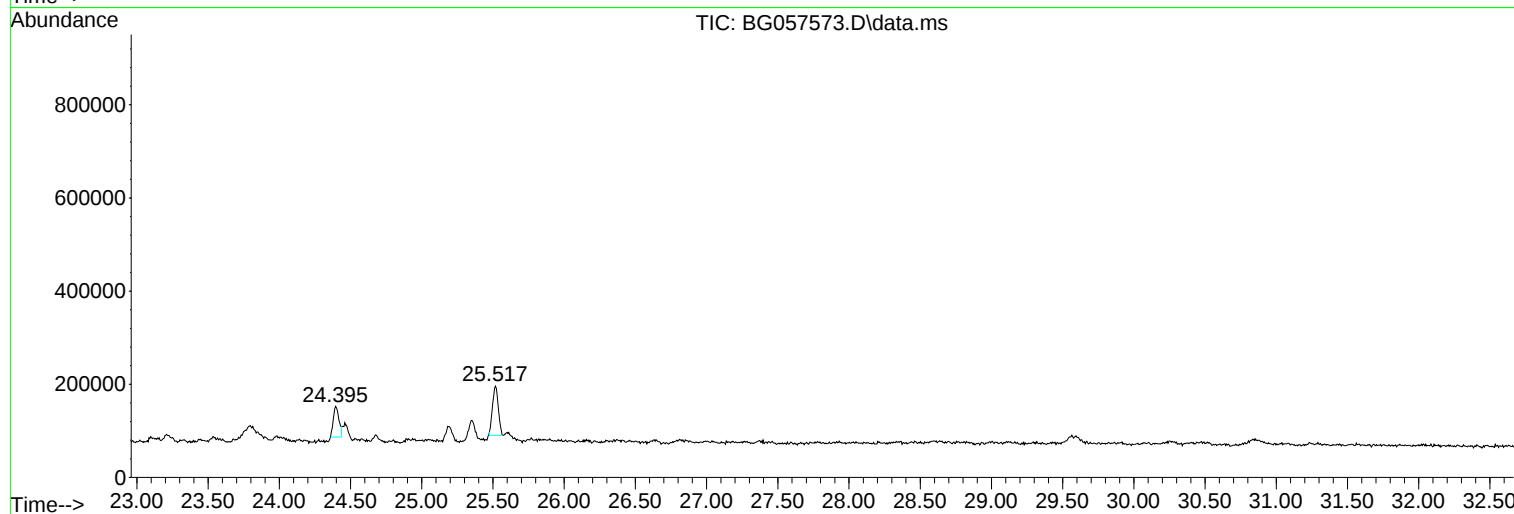
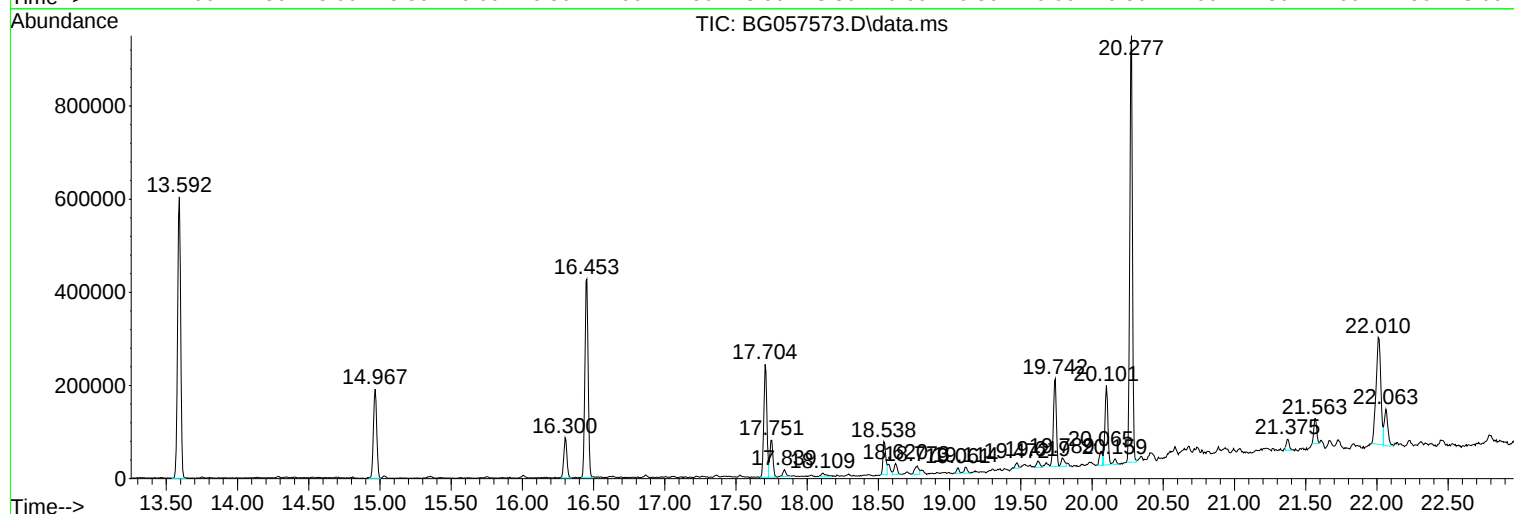
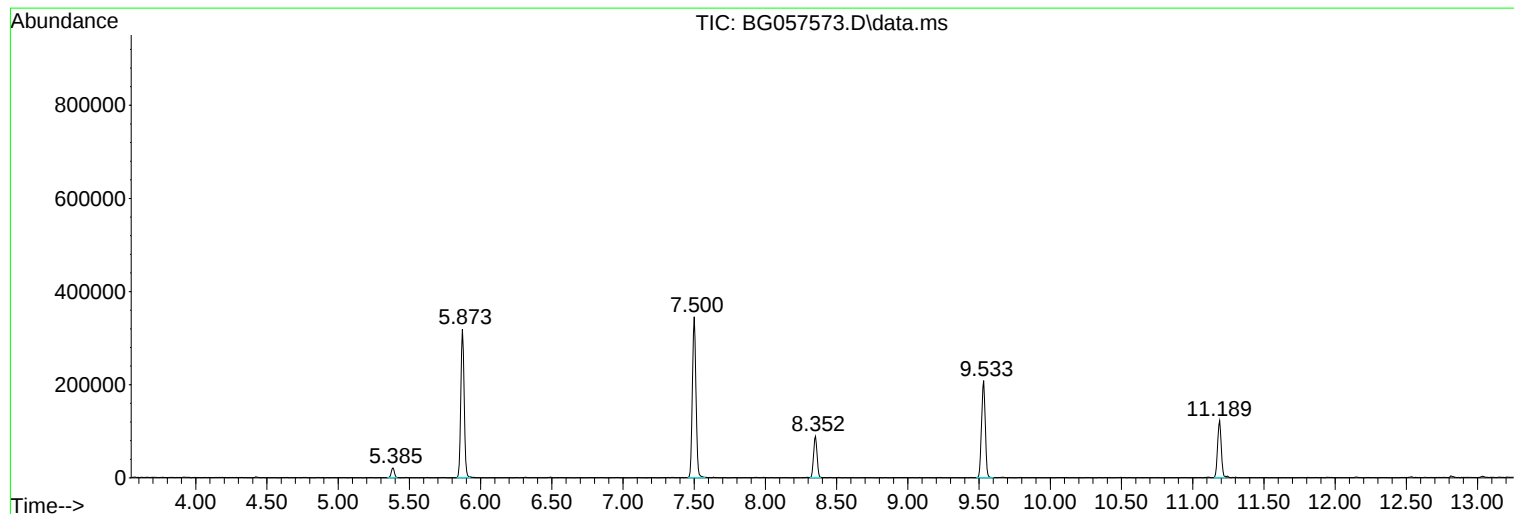
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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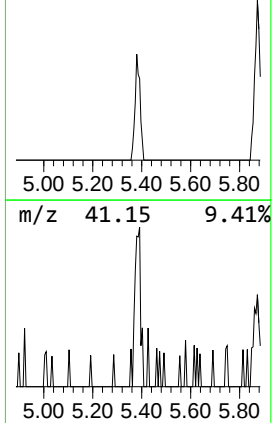
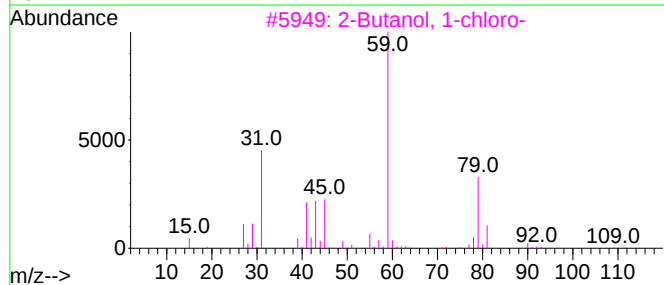
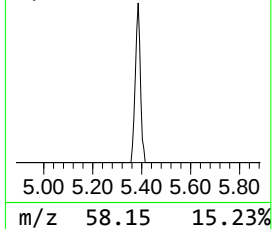
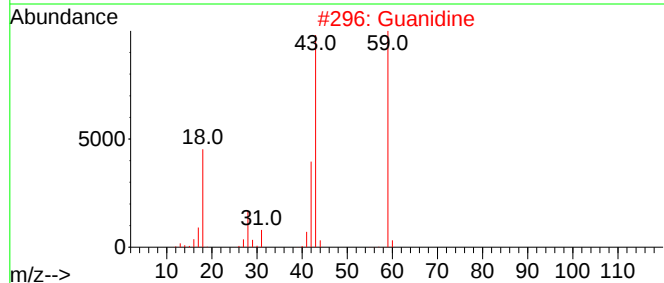
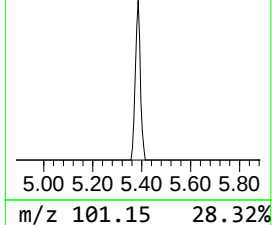
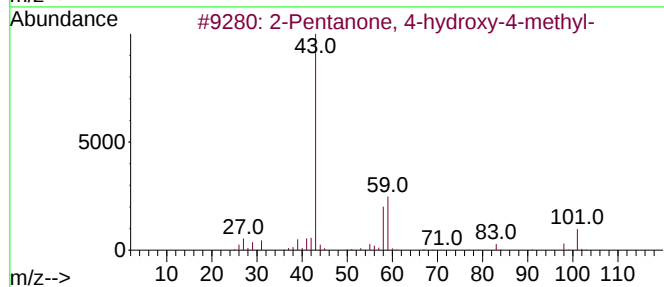
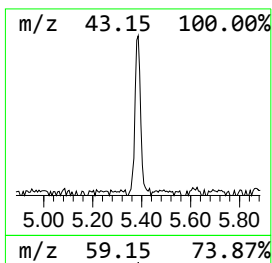
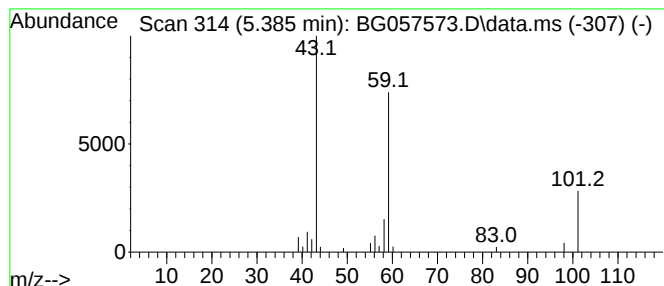
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.385	4.41 ng	32871	1,4-Dichlorobenzene-d4	8.352

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	Guanidine	59	CH5N3	000113-00-8	50	
3	2-Butanol, 1-chloro-	108	C4H9ClO	001873-25-2	28	
4	3-Pentanol	88	C5H12O	000584-02-1	9	
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9	



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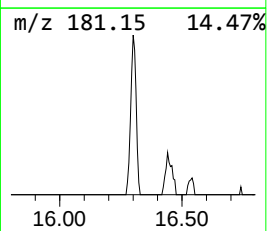
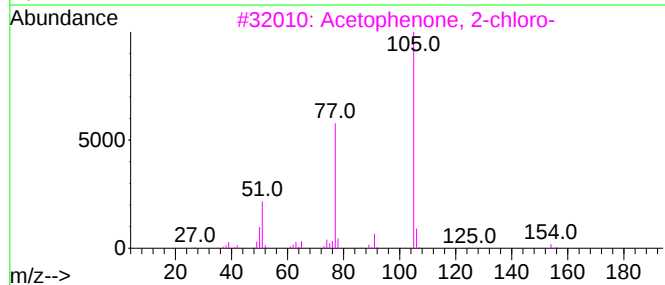
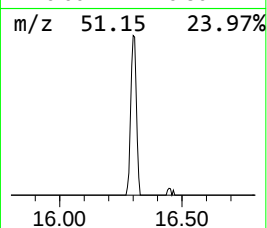
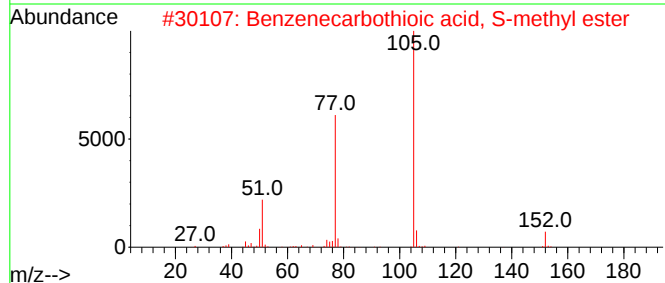
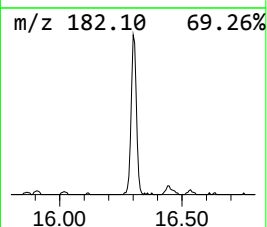
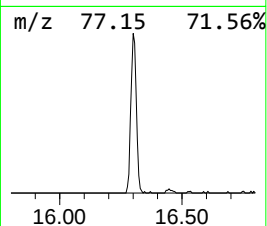
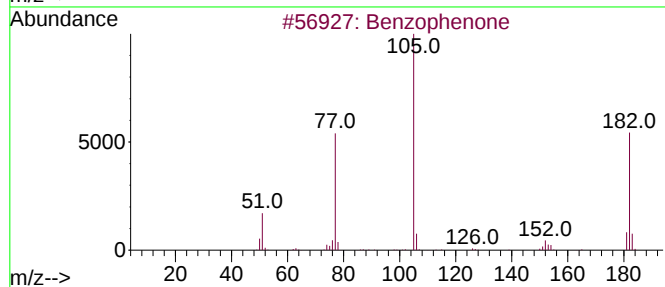
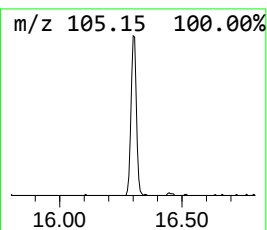
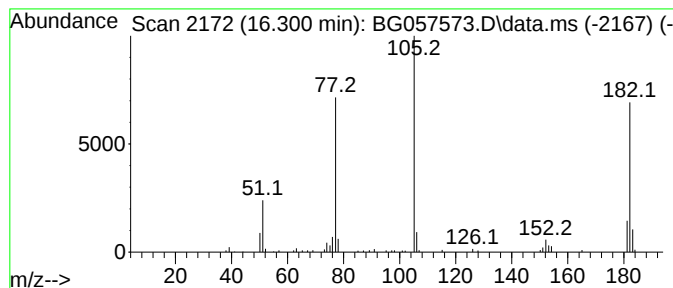
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.300	8.51 ng	131293	Acenaphthene-d10	14.967

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4			Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	43
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	43



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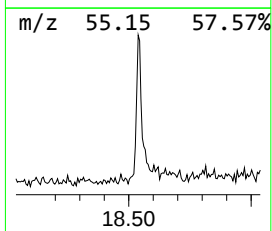
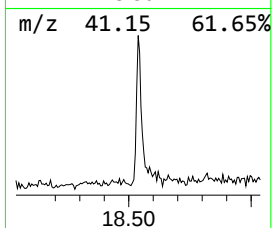
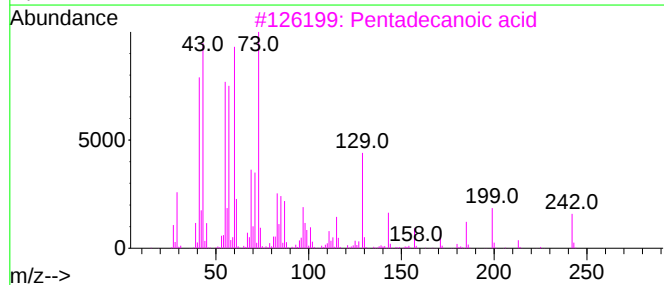
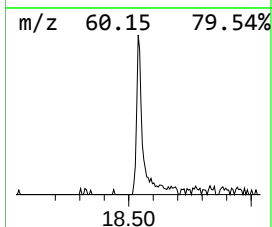
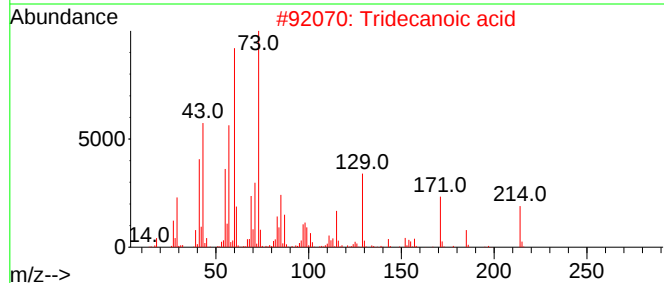
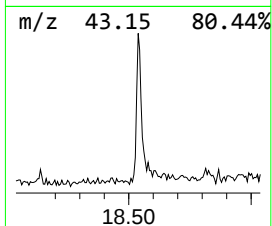
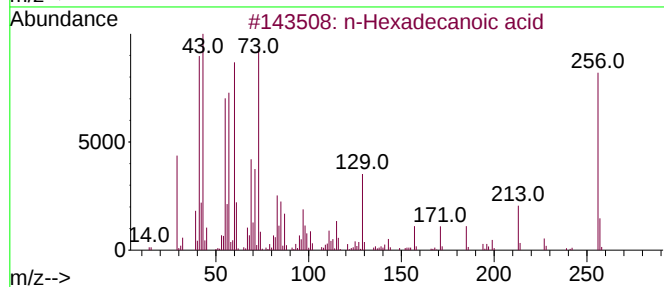
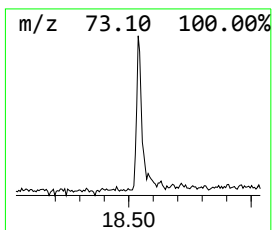
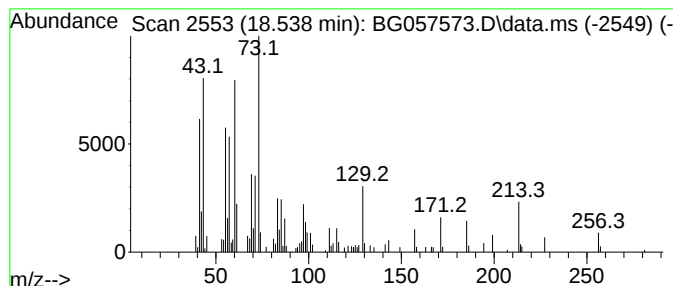
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.538	5.42 ng	99142	Phenanthrene-d10	17.704	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



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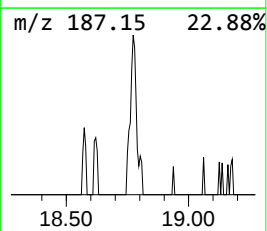
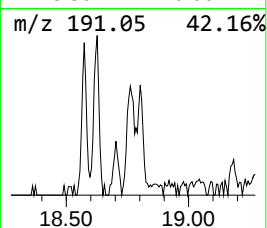
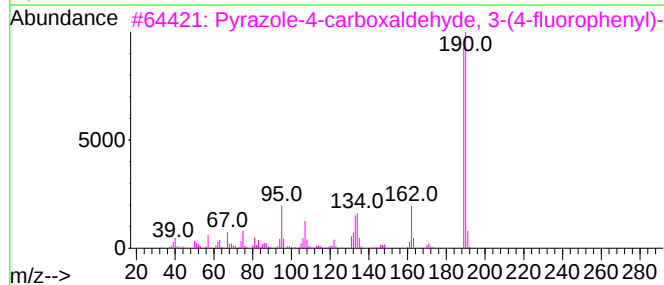
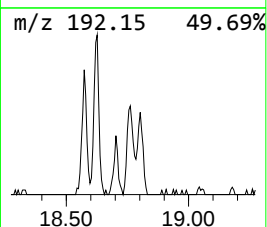
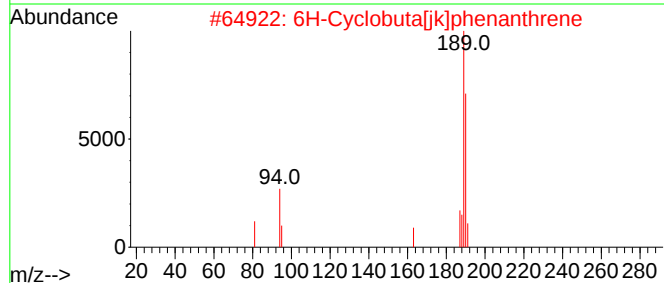
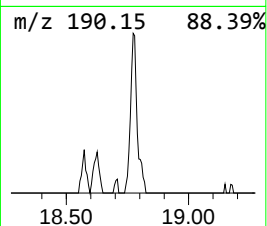
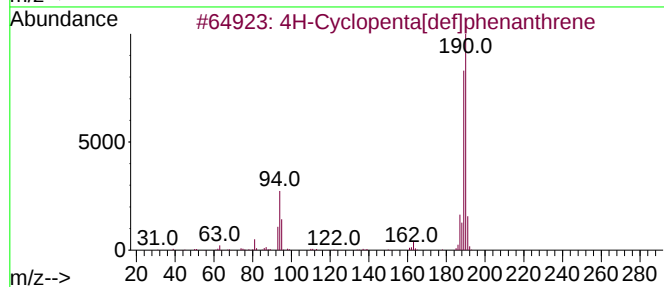
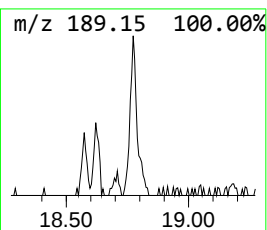
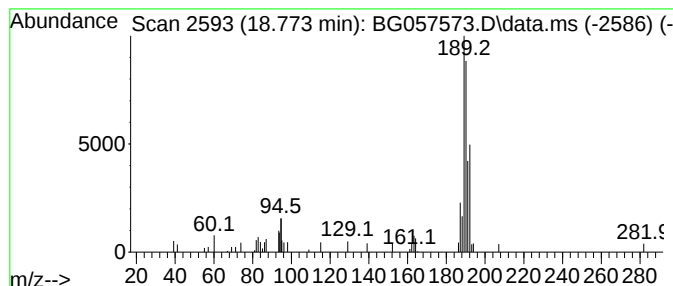
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.773	2.04 ng	37300	Phenanthrene-d10	17.704	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	62
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	46
4	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	38
5	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	37



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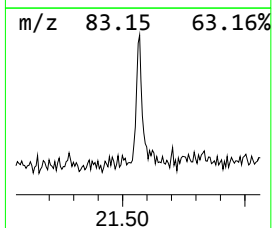
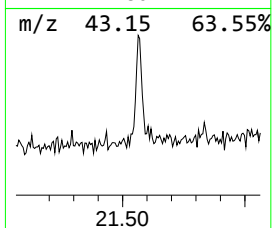
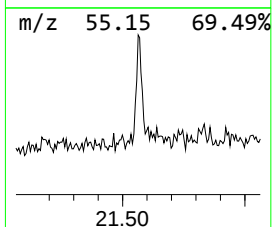
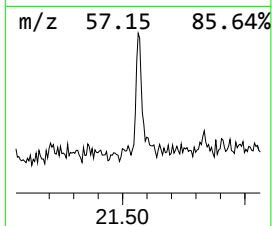
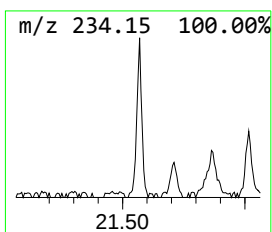
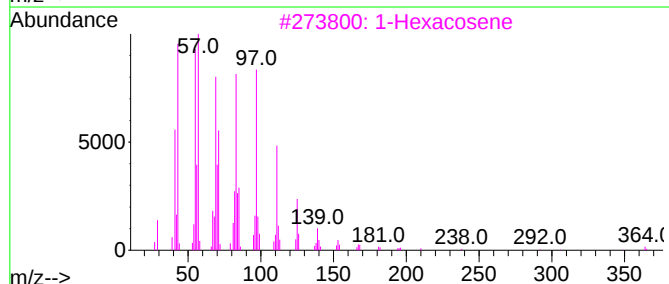
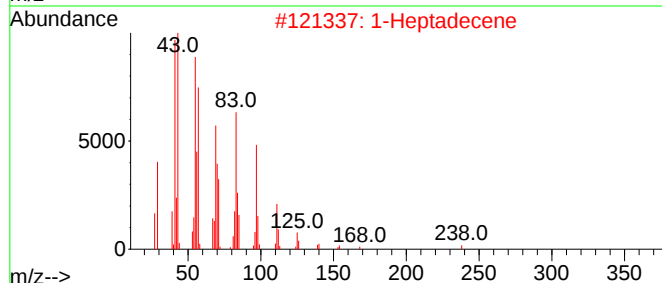
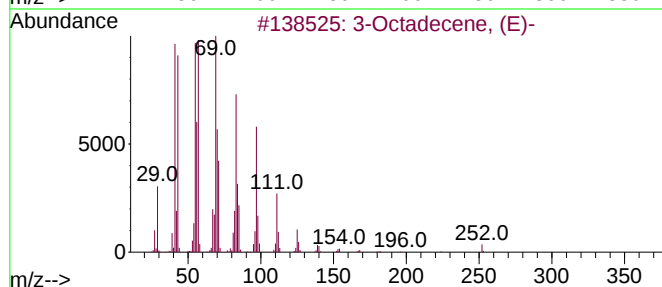
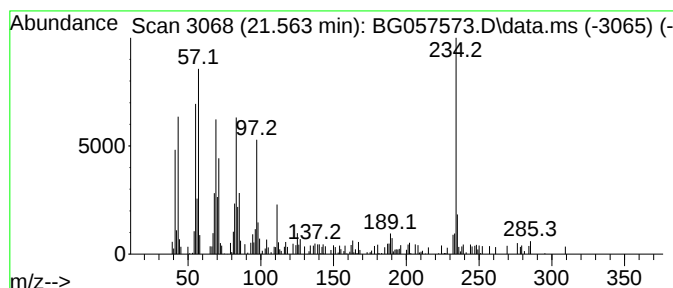
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Peak Number 5 3-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.564	2.92 ng	78102	Chrysene-d12	22.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Octadecene, (E)-	252	C18H36	007206-19-1	64
2		1-Heptadecene	238	C17H34	006765-39-5	64
3		1-Hexacosene	364	C26H52	018835-33-1	60
4		17-Pentatriacontene	491	C35H70	006971-40-0	53
5		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	53



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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
2-Pentanone, 4-...	5.385	4.4	ng	32871	1	8.352	149229	20.0
Benzophenone	16.300	8.5	ng	131293	3	14.967	308697	20.0
n-Hexadecanoic ...	18.538	5.4	ng	99142	4	17.704	365904	20.0
4H-Cyclopenta[d...]	18.773	2.0	ng	37300	4	17.704	365904	20.0
3-Octadecene, (E)-	21.564	2.9	ng	78102	5	22.016	534921	20.0