

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020723\
 Data File : BG056570.D
 Acq On : 7 Feb 2023 16:40
 Operator : CG/JU
 Sample : 01463-12
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-6

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-BG012723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056570.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.303	336	343	350	rBV	119006	180892	7.01%	1.477%
2	5.791	419	426	437	rBV	470922	764183	29.62%	6.241%
3	7.419	694	703	714	rBV	476689	818951	31.74%	6.689%
4	8.271	841	848	854	rBB	116131	195390	7.57%	1.596%
5	9.446	1040	1048	1056	rBV	278372	500014	19.38%	4.084%
6	11.102	1322	1330	1338	rBV	156439	283516	10.99%	2.316%
7	13.511	1733	1740	1747	rBV	1108547	1685537	65.32%	13.767%
8	14.886	1968	1974	1981	rVB	296525	457406	17.73%	3.736%
9	16.226	2196	2202	2208	rBV	45431	66500	2.58%	0.543%
10	16.373	2220	2227	2235	rBV	804909	1185216	45.93%	9.680%
11	17.630	2432	2441	2445	rBV	389130	588133	22.79%	4.804%
12	17.671	2445	2448	2453	rVB	69614	96592	3.74%	0.789%
13	18.476	2579	2585	2592	rBV3	62721	114446	4.44%	0.935%
14	18.547	2592	2597	2603	rVB2	21805	35245	1.37%	0.288%
15	18.694	2615	2622	2625	rBV2	22597	39818	1.54%	0.325%
16	19.663	2781	2787	2792	rBV	186363	253085	9.81%	2.067%
17	19.986	2838	2842	2844	rBV2	23008	33201	1.29%	0.271%
18	20.021	2844	2848	2854	rVB	169365	232893	9.03%	1.902%
19	20.204	2873	2879	2885	rBV	2038593	2580370	100.00%	21.075%
20	20.345	2897	2903	2908	rVB5	14831	34920	1.35%	0.285%
21	20.503	2928	2930	2935	rVB2	27200	33837	1.31%	0.276%
22	21.490	3094	3098	3109	rVB3	67592	135476	5.25%	1.106%
23	21.913	3162	3170	3176	rBV3	387282	790764	30.65%	6.459%
24	21.966	3176	3179	3185	rVB	65563	97195	3.77%	0.794%
25	23.629	3457	3462	3467	rVB	48063	85343	3.31%	0.697%
26	24.240	3561	3566	3576	rBV	45028	149153	5.78%	1.218%
27	25.016	3694	3698	3705	rVB2	30388	68819	2.67%	0.562%
28	25.168	3719	3724	3736	rVB	52916	152014	5.89%	1.242%
29	25.339	3744	3753	3761	rVB2	210236	584796	22.66%	4.776%

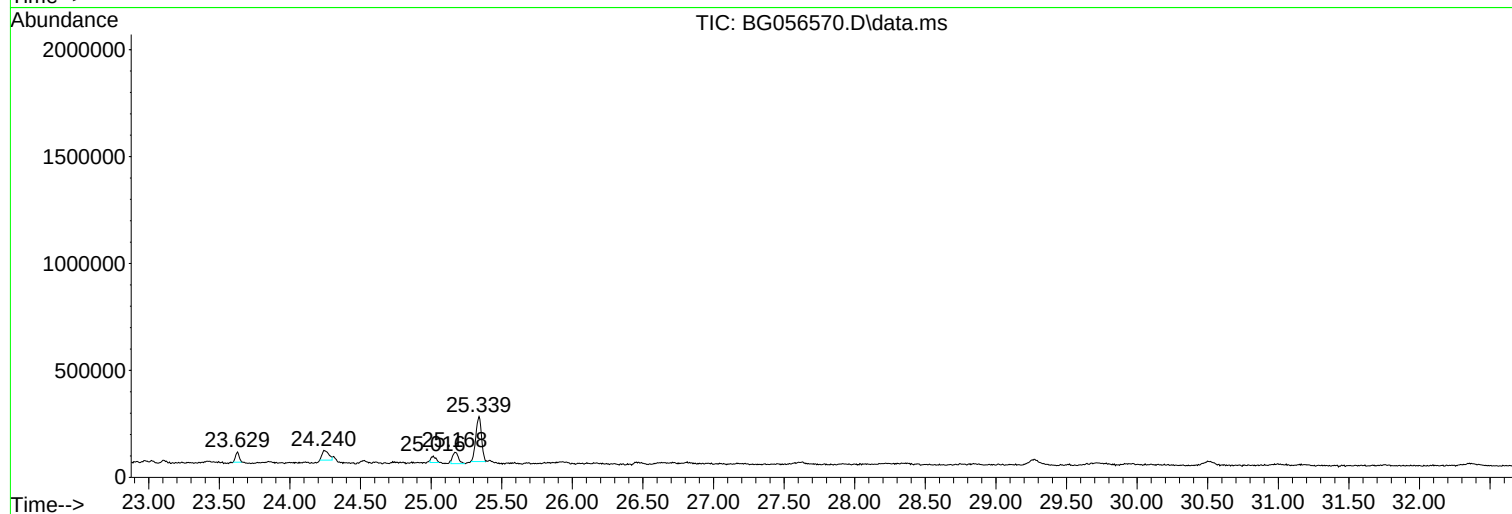
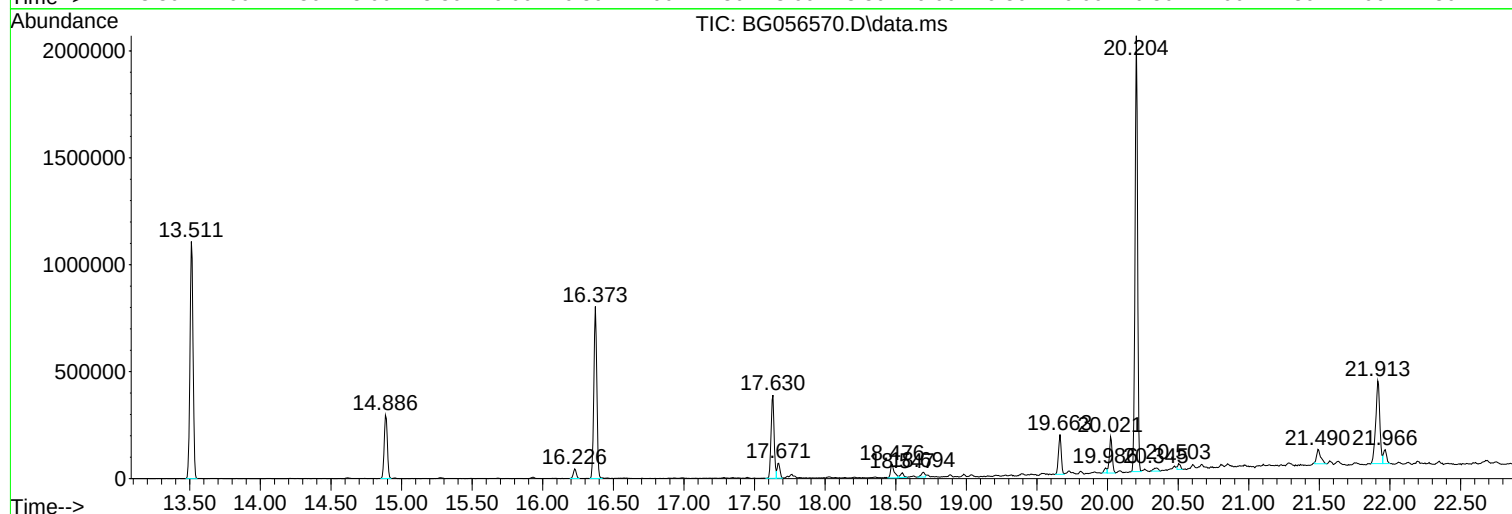
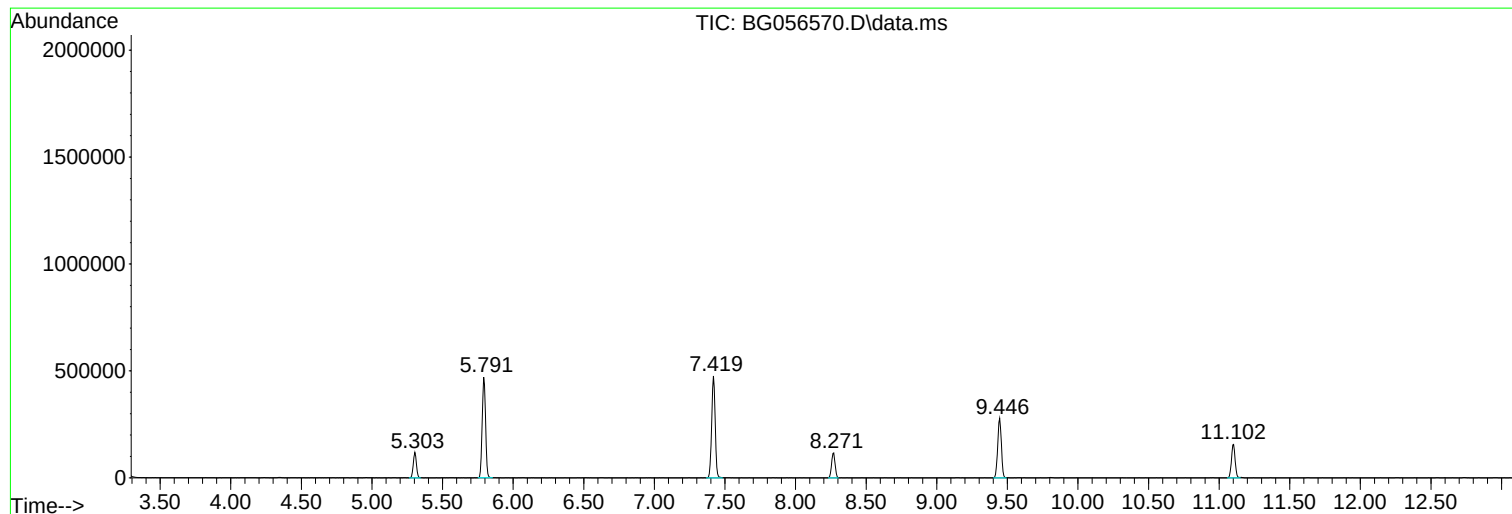
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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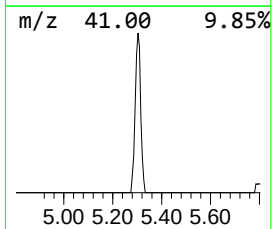
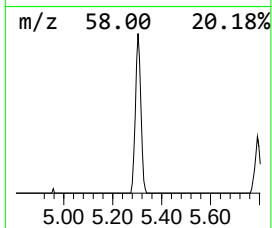
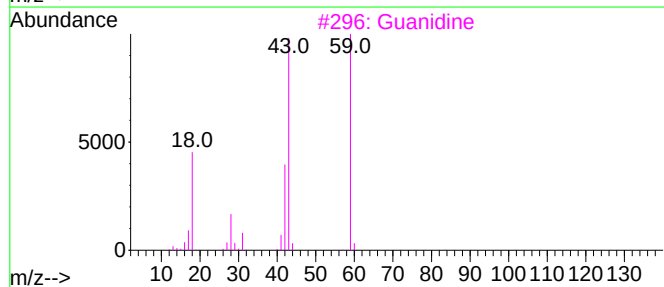
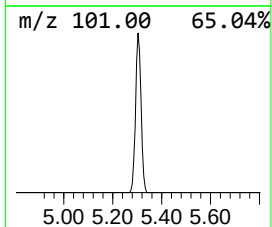
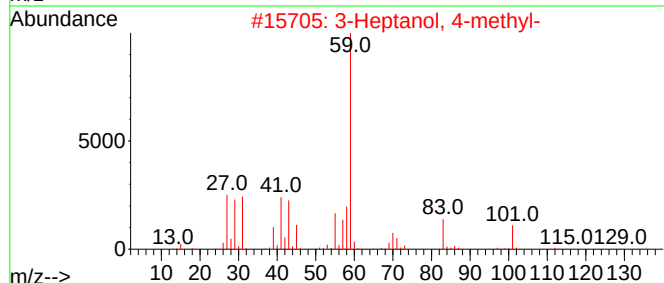
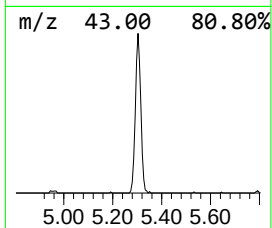
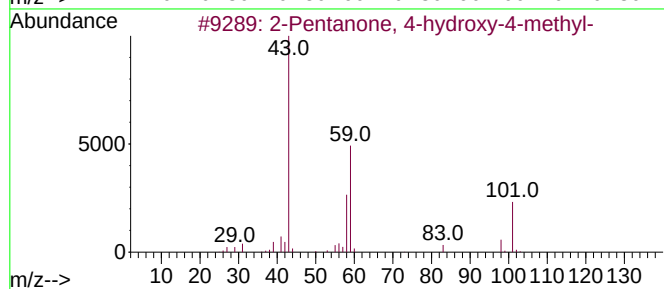
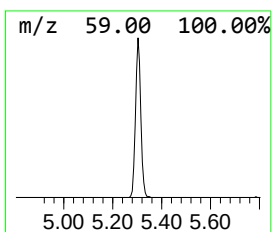
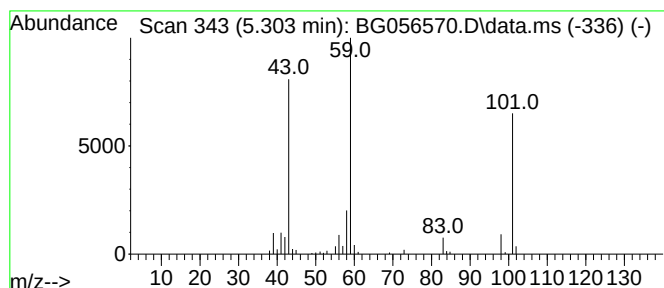
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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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.
5.303	18.52 ng	180892	1,4-Dichlorobenzene-d4	8.271

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28		
3	Guanidine	59	CH5N3	000113-00-8	25		
4	6-Nitrohexan-2-ol	147	C6H13NO3	062224-53-7	25		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25		



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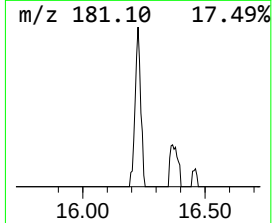
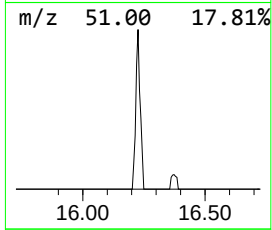
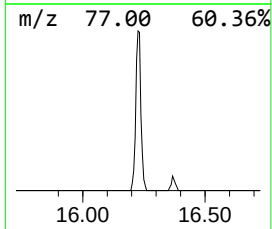
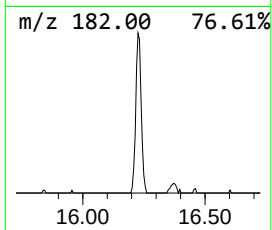
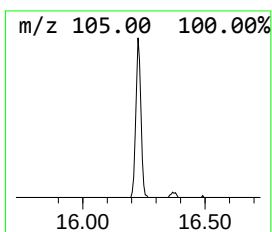
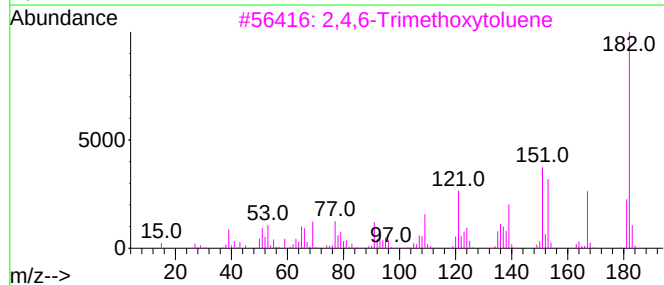
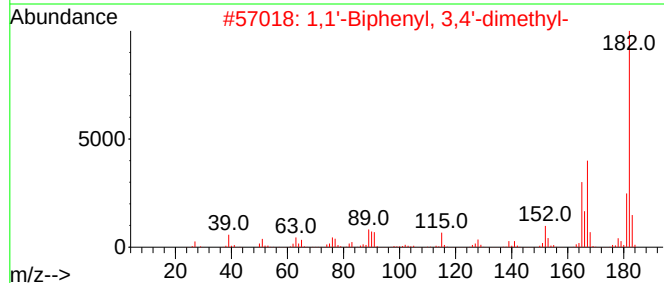
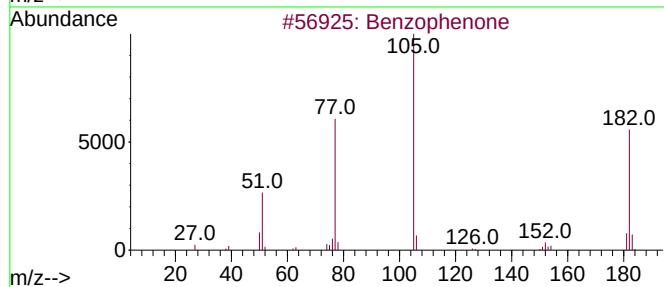
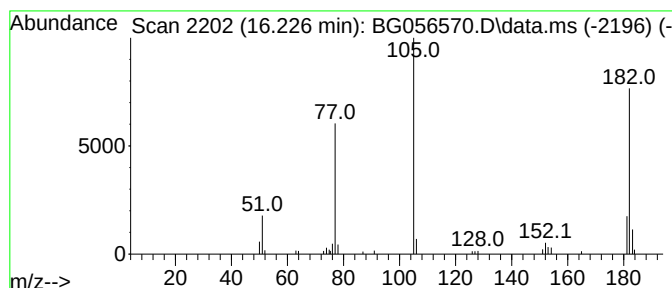
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.226	2.91 ng	66500	Acenaphthene-d10	14.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	46
3			2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	43
4			9H-Pyrido[3,4-b]indole, 1-methyl-	182	C12H10N2	000486-84-0	43
5			3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43



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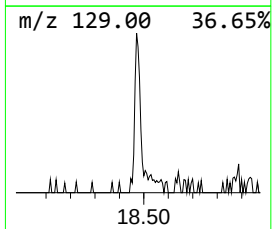
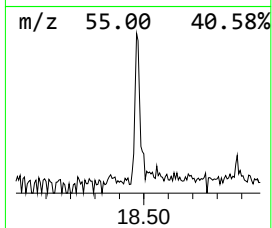
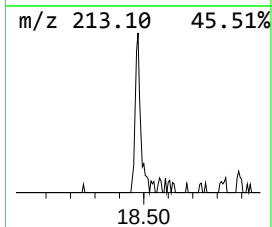
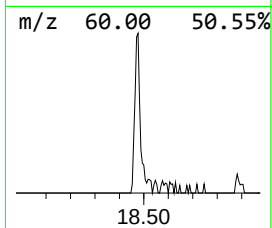
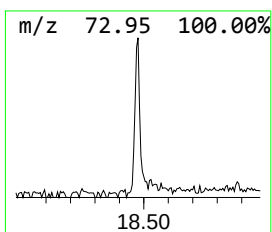
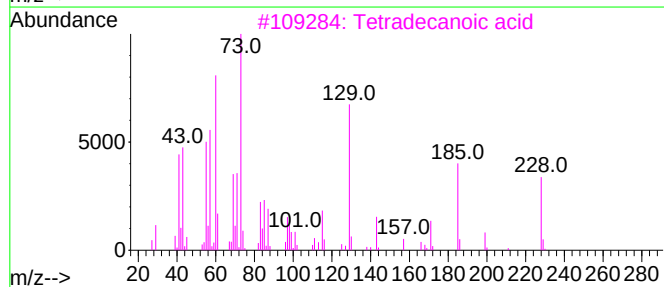
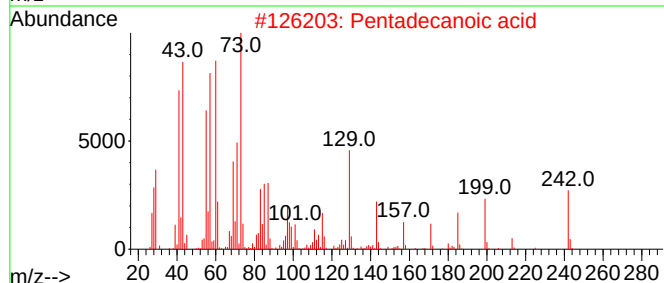
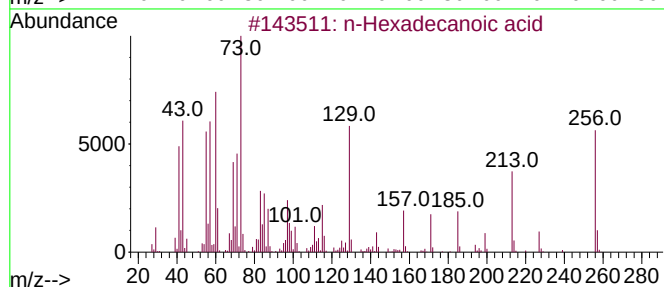
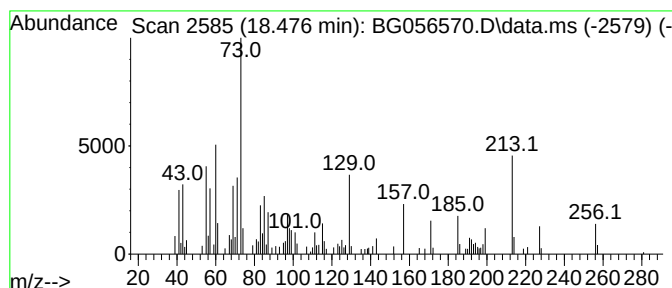
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.476	3.89 ng	114446	Phenanthrene-d10		17.630	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	46
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	46
4	n-Decanoic acid		172	C10H20O2	000334-48-5	42
5	Tridecanoic acid		214	C13H26O2	000638-53-9	38



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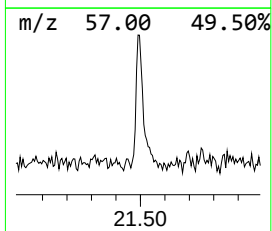
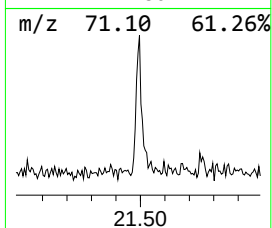
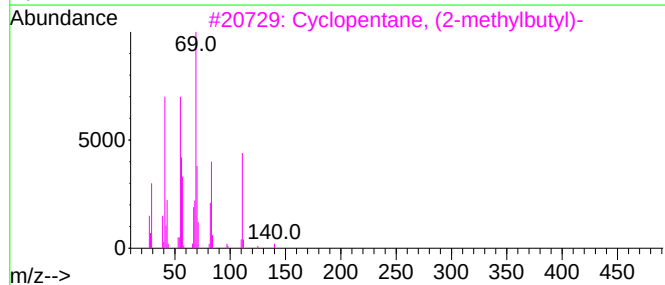
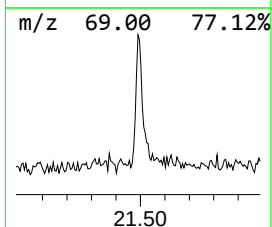
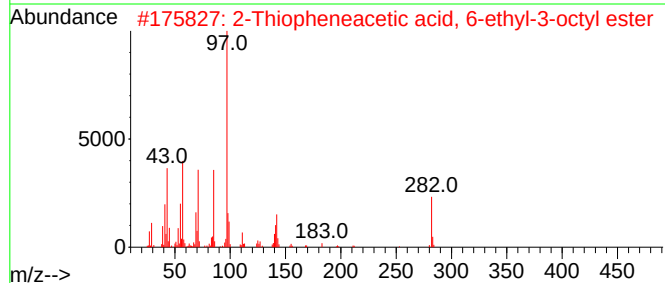
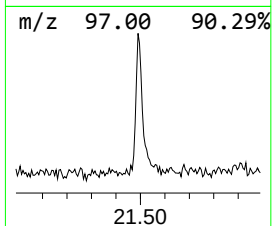
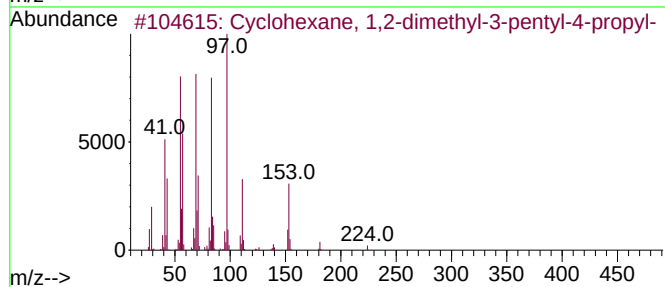
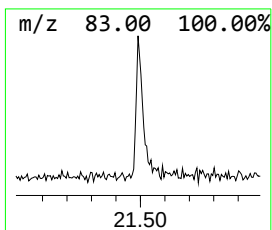
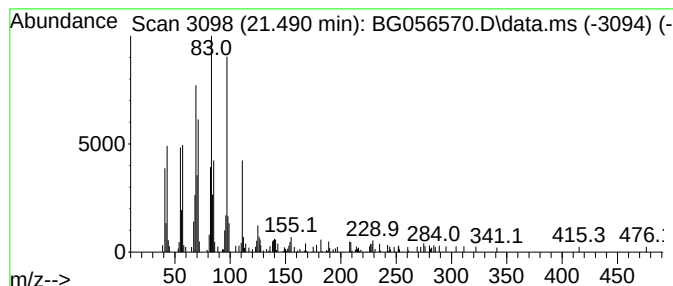
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Peak Number 4 Cyclohexane, 1,2-dimethyl-3... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.490	3.43 ng	135476	Chrysene-d12	21.913

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	53
2			2-Thiopheneacetic acid, 6-ethyl-...	282	C16H26O2S	1000278-92-3	38
3			Cyclopentane, (2-methylbutyl)-	140	C10H20	053366-38-4	35
4			1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	27
5			2-Thiopheneacetic acid, 3,5-dime...	252	C14H20O2S	1000278-92-2	25



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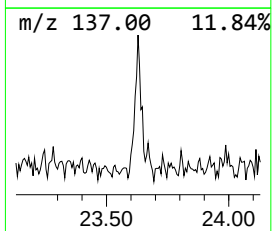
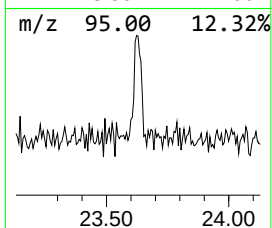
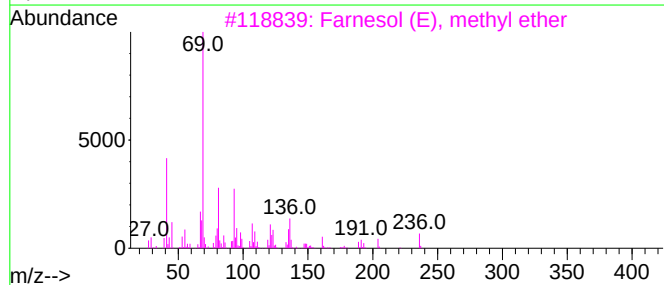
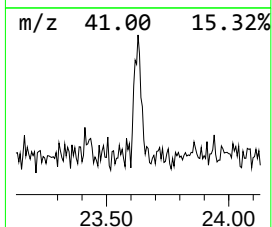
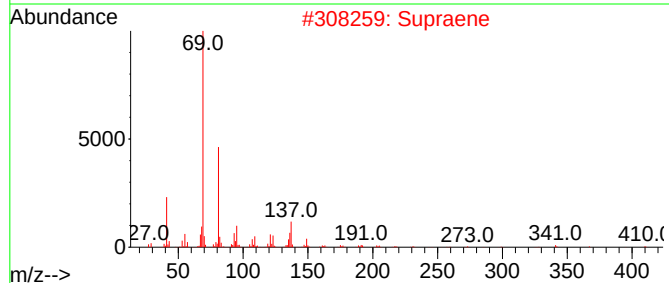
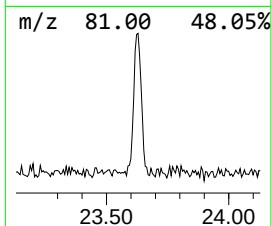
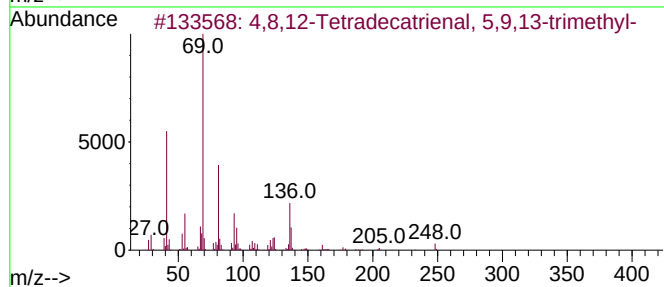
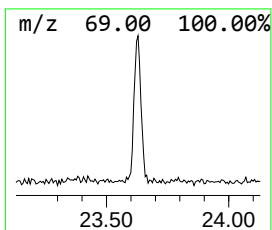
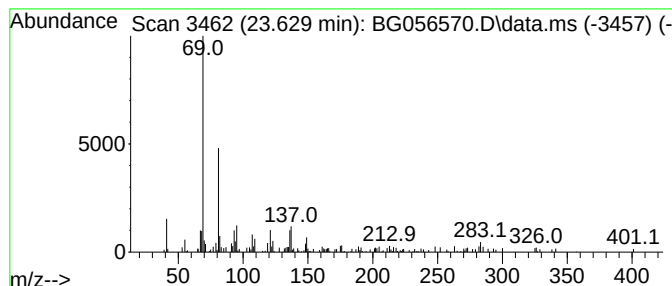
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Peak Number 5 4,8,12-Tetradecatrienal, 5,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.629	2.92 ng	85343	Perylene-d12	25.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	81		
2	Supraene	410	C30H50	007683-64-9	78		
3	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72		
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72		
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	53		



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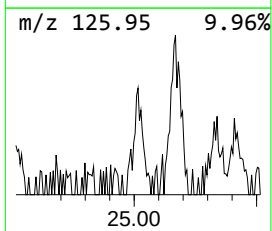
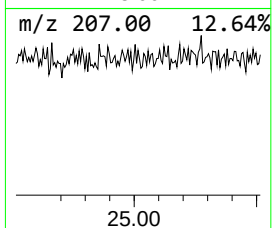
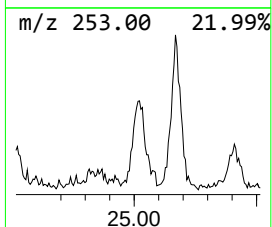
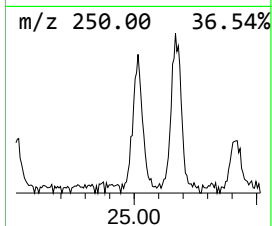
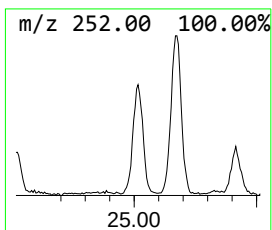
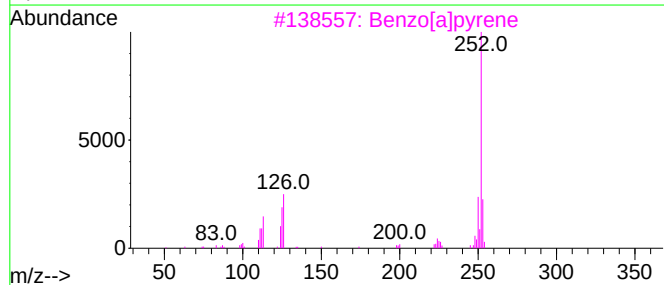
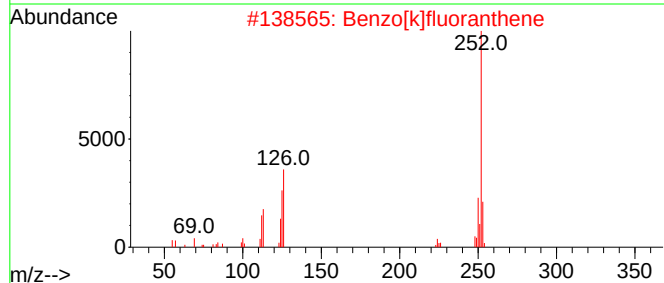
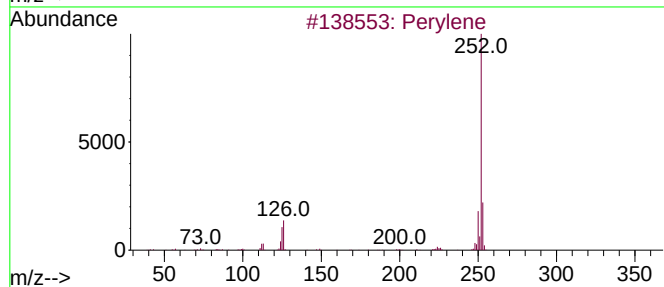
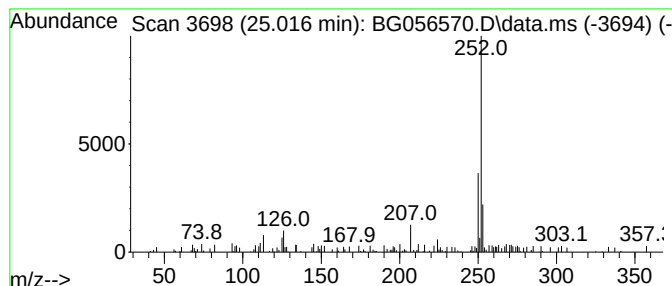
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.016	2.35 ng	68819	Perylene-d12	25.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	58
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	53
3			Benzo[a]pyrene	252	C20H12	000050-32-8	53
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	52
5			1-Phenyl-3-(4-methoxyphenyl)-2-p...	252	C16H16N2O	003314-43-0	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020723\
Data File : BG056570.D
Acq On : 7 Feb 2023 16:40
Operator : CG/JU
Sample : 01463-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG012723.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-...	5.303	18.5	ng	180892	1	8.271	195390	20.0
Benzophenone	16.226	2.9	ng	66500	3	14.886	457406	20.0
n-Hexadecanoic ...	18.476	3.9	ng	114446	4	17.630	588133	20.0
Cyclohexane, 1,...	21.490	3.4	ng	135476	5	21.913	790764	20.0
4,8,12-Tetradec...	23.629	2.9	ng	85343	6	25.339	584796	20.0
Perylene	25.016	2.4	ng	68819	6	25.339	584796	20.0