

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012023\
 Data File : BG056378.D
 Acq On : 20 Jan 2023 22:13
 Operator : CG/JU
 Sample : 01229-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 OK-02-011923

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.348	343	350	362	rBV	112154	198156	10.54%	1.764%
2	5.835	424	433	448	rBV	479240	879778	46.81%	7.830%
3	7.451	700	708	722	rBV	503568	951866	50.65%	8.472%
4	8.309	849	854	870	rVB	159593	281103	14.96%	2.502%
5	8.873	944	950	957	rVB6	11027	24185	1.29%	0.215%
6	9.161	993	999	1002	rBV5	9879	20969	1.12%	0.187%
7	9.414	1032	1042	1047	rBV7	16862	43246	2.30%	0.385%
8	9.484	1047	1054	1067	rVB	312633	629866	33.51%	5.606%
9	10.048	1146	1150	1159	rVB5	8834	19666	1.05%	0.175%
10	11.141	1329	1336	1343	rBV	197927	368774	19.62%	3.282%
11	12.774	1608	1614	1621	rVB2	12282	20676	1.10%	0.184%
12	12.998	1642	1652	1659	rBV4	11510	32750	1.74%	0.291%
13	13.550	1738	1746	1757	rBV	1008114	1586870	84.43%	14.123%
14	14.102	1833	1840	1845	rVB9	8698	22011	1.17%	0.196%
15	14.243	1859	1864	1868	rBV4	16778	25288	1.35%	0.225%
16	14.925	1974	1980	1986	rVB	346342	545925	29.05%	4.859%
17	15.307	2043	2045	2051	rVB4	14203	21549	1.15%	0.192%
18	15.959	2152	2156	2161	rBV4	17093	30250	1.61%	0.269%
19	16.259	2202	2207	2214	rVB	137886	199197	10.60%	1.773%
20	16.405	2226	2232	2240	rBV	770233	1176853	62.62%	10.474%
21	17.316	2383	2387	2390	rBV5	15129	24551	1.31%	0.219%
22	17.663	2440	2446	2450	rBV	410877	647200	34.44%	5.760%
23	17.704	2450	2453	2459	rVB	192092	275273	14.65%	2.450%
24	18.509	2586	2590	2592	rBV	85408	122692	6.53%	1.092%
25	18.579	2599	2602	2608	rVB	75528	104242	5.55%	0.928%
26	18.714	2623	2625	2630	rBV2	39927	66892	3.56%	0.595%
27	19.696	2787	2792	2797	rBV	354934	520668	27.70%	4.634%
28	20.054	2850	2853	2860	rVB	340791	515742	27.44%	4.590%
29	20.236	2879	2884	2889	rBV	1479909	1879448	100.00%	16.727%

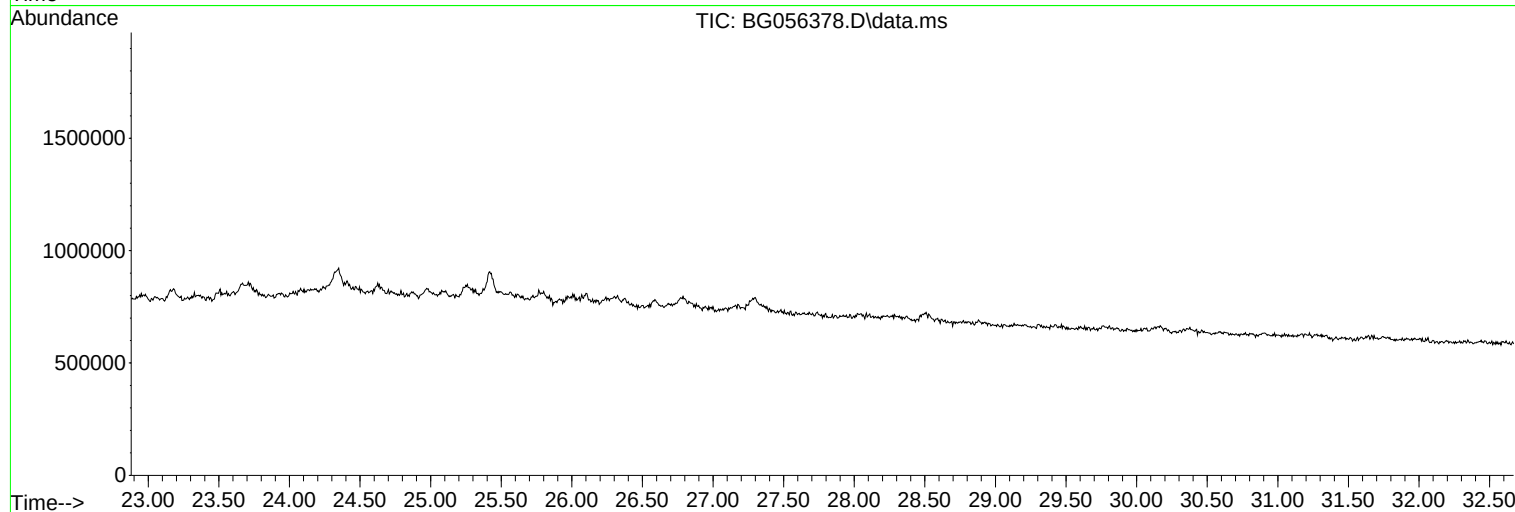
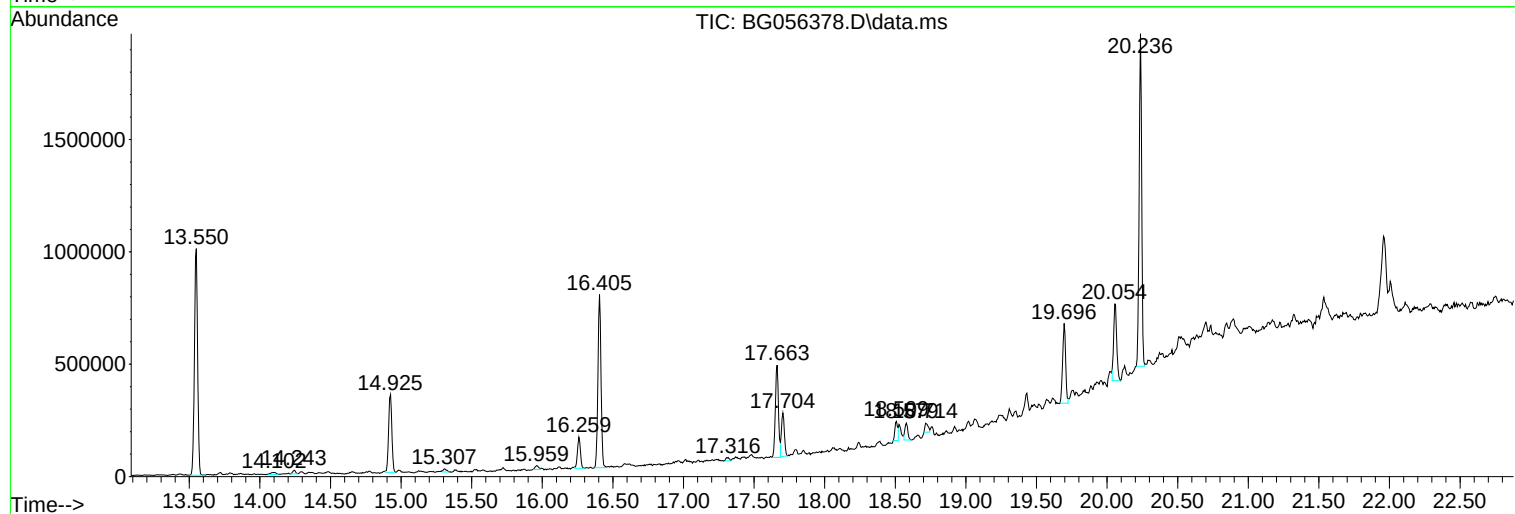
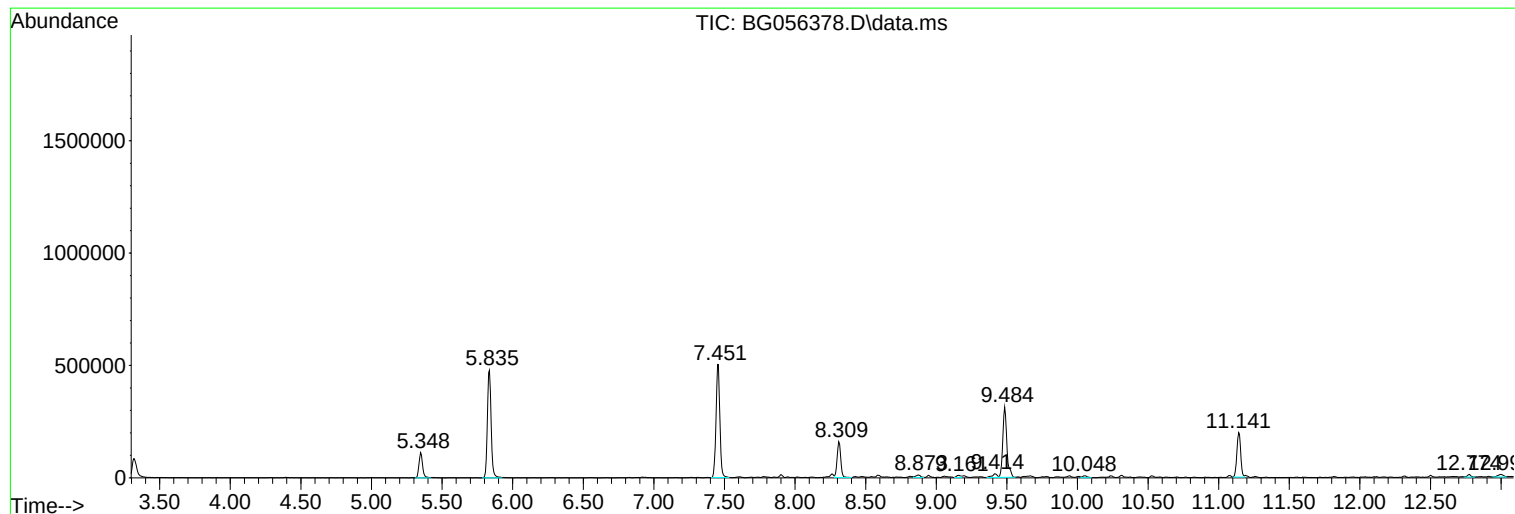
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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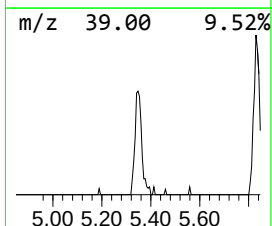
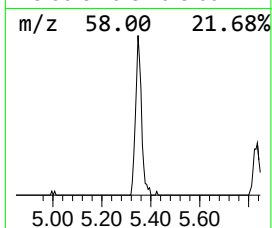
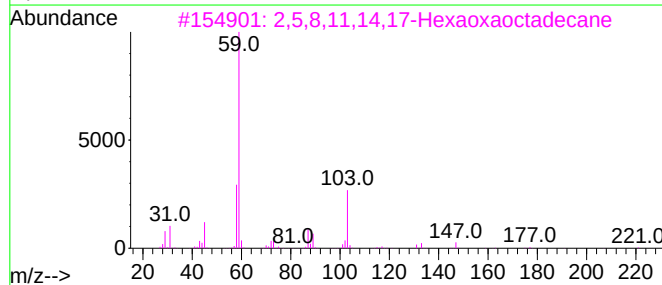
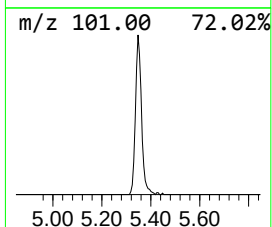
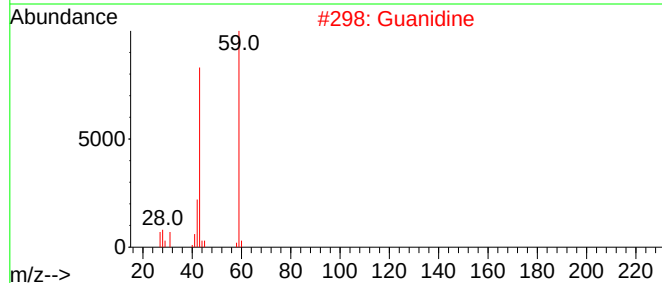
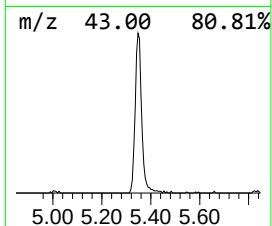
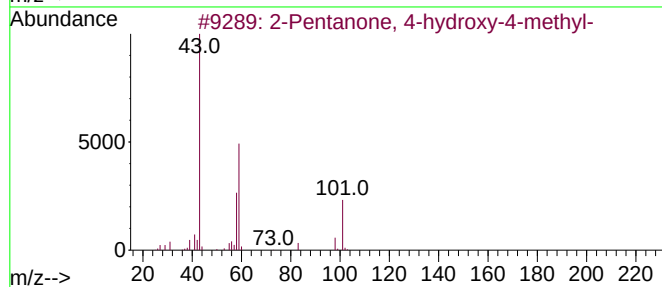
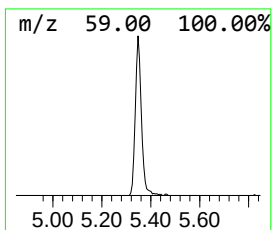
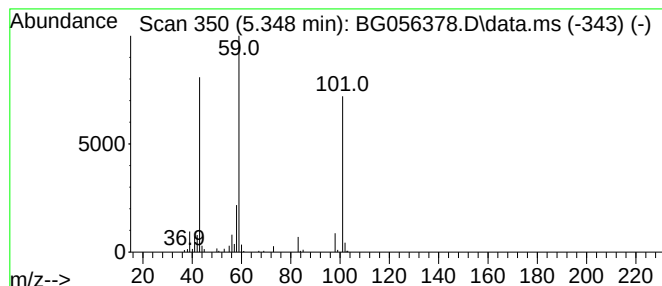
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.348	14.10 ng	198156	1,4-Dichlorobenzene-d4	8.309

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38		
2	Guanidine	59	CH5N3	000113-00-8	37		
3	2,5,8,11,14,17-Hexaoxaoctadecane	266	C12H26O6	001191-87-3	28		
4	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	25		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



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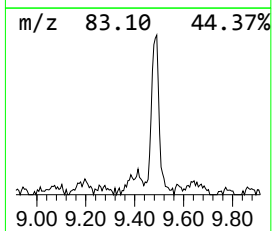
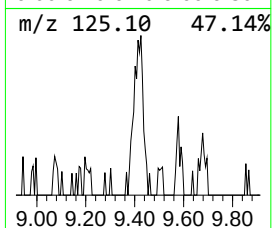
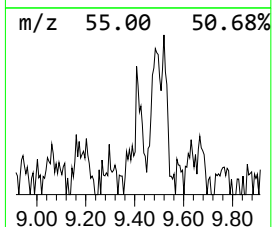
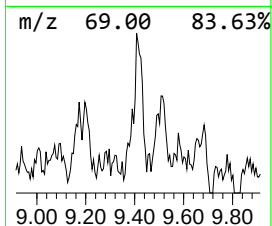
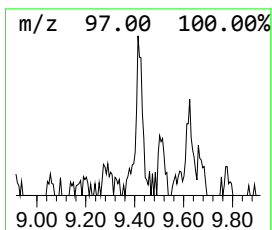
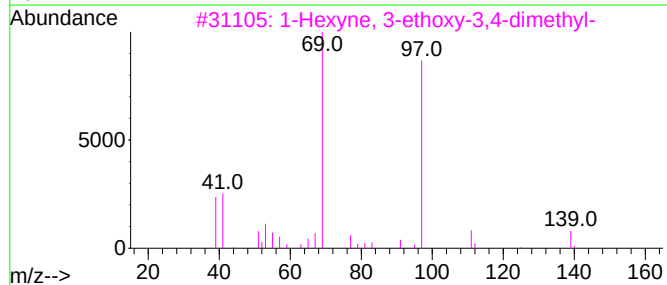
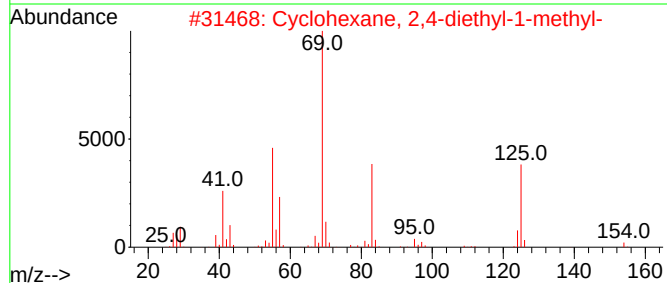
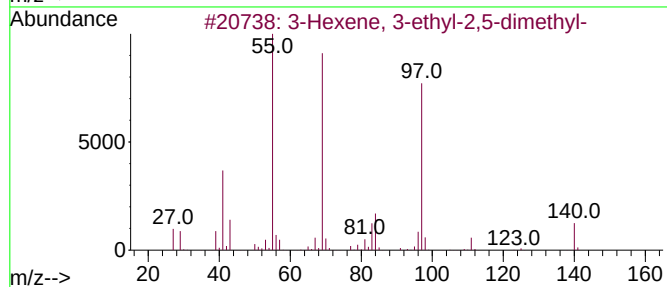
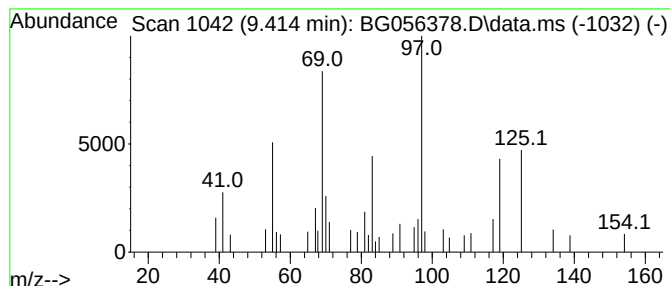
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown9.414 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.414	3.08 ng	43246	1,4-Dichlorobenzene-d4	8.309

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	43
2		Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	38
3		1-Hexyne, 3-ethoxy-3,4-dimethyl-	154	C10H18O	054244-91-6	35
4		Cyclohexane, 1,1'-(1-methylethyl...	208	C15H28	054934-90-6	27
5		Cyclopentane, hexyl-	154	C11H22	004457-00-5	25



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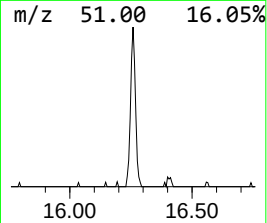
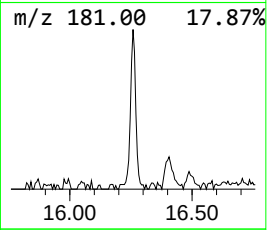
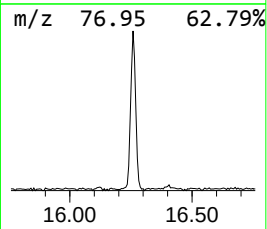
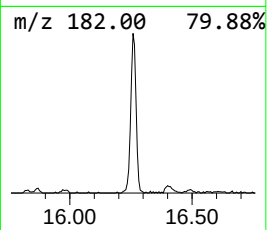
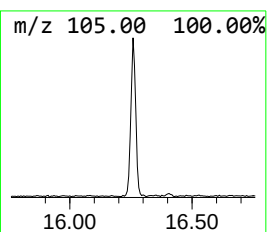
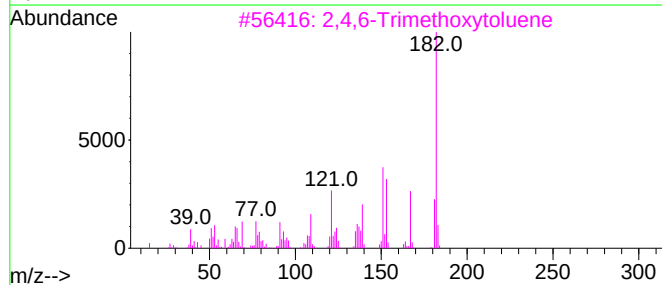
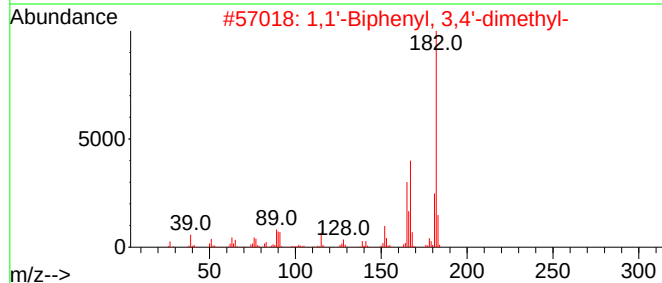
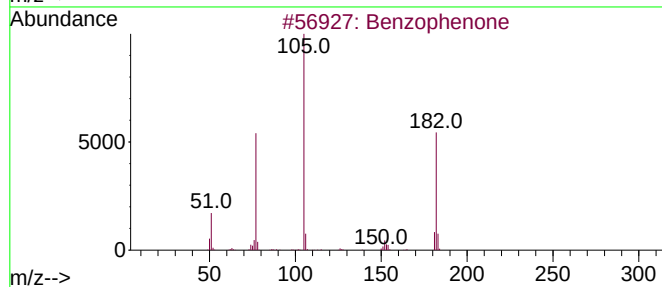
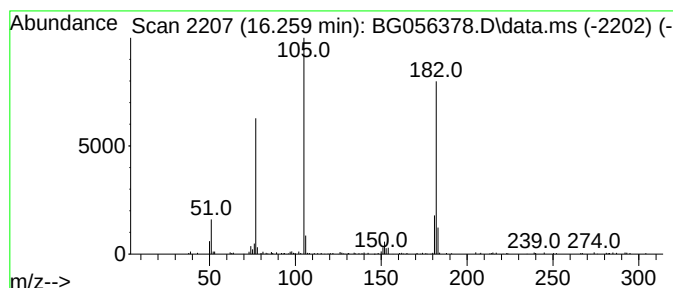
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.259	7.30 ng	199197	Acenaphthene-d10		14.925	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzophenone		182	C13H10O	000119-61-9	96
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	3,3'-Dimethylbiphenyl		182	C14H14	000612-75-9	43
5	4,4'-Dimethylbiphenyl		182	C14H14	000613-33-2	43



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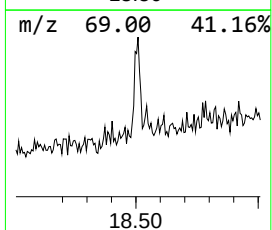
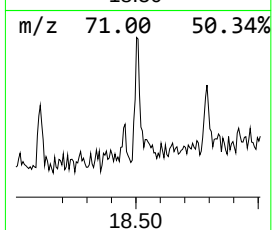
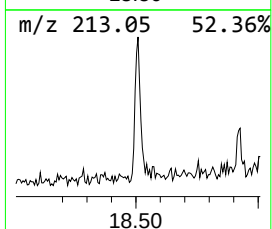
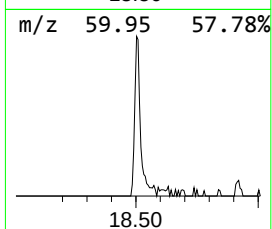
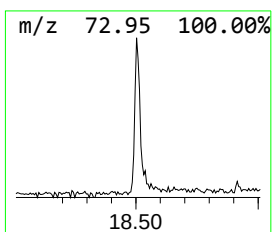
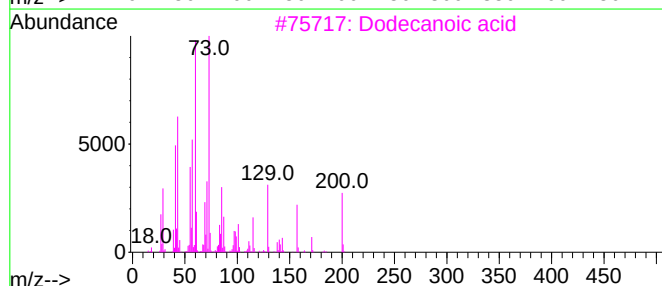
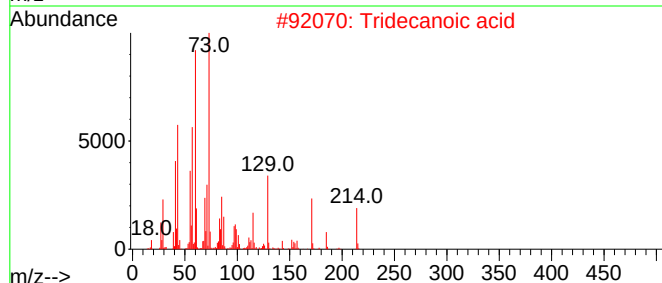
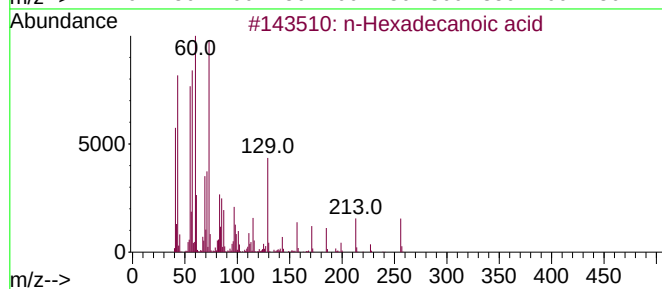
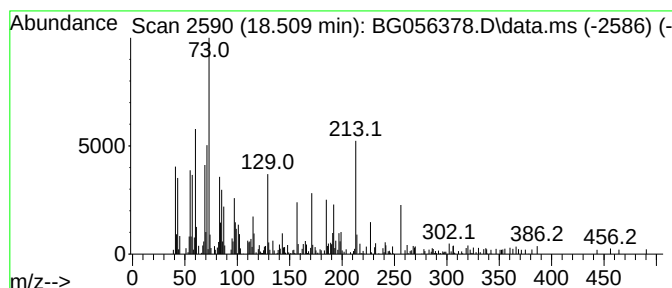
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.509	3.79 ng	122692	Phenanthrene-d10	17.663	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
2	Tridecanoic acid	214	C13H26O2	000638-53-9	52
3	Dodecanoic acid	200	C12H24O2	000143-07-7	46
4	Tetracosanoic acid	368	C24H48O2	000557-59-5	38
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	38



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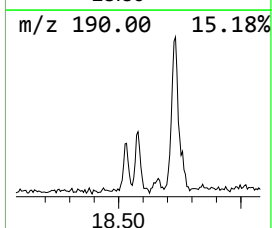
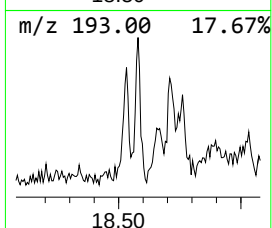
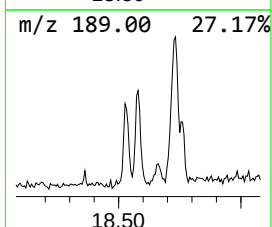
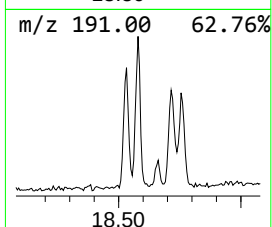
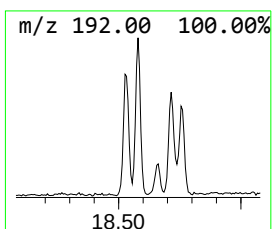
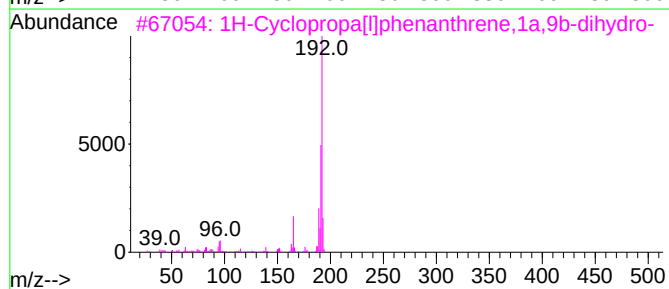
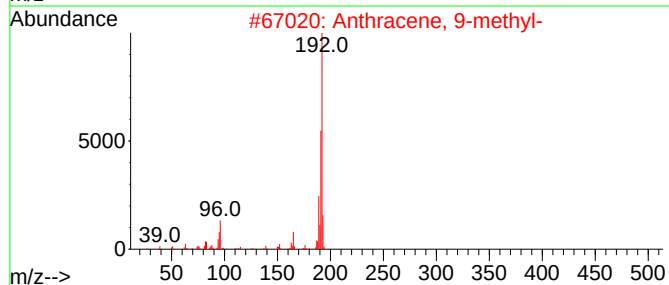
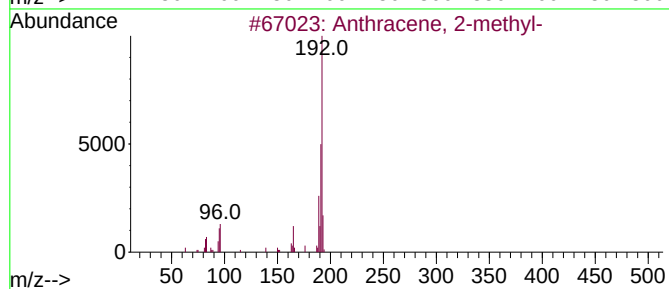
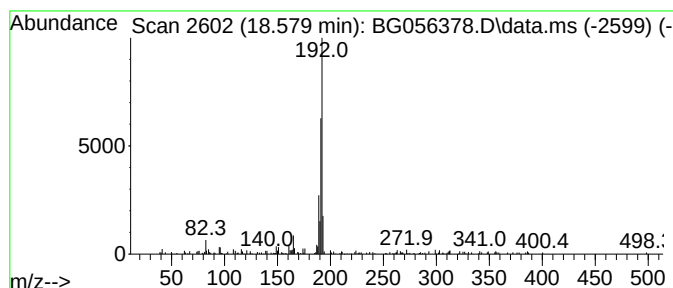
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Anthracene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.579	3.22 ng	104242	Phenanthrene-d10	17.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
3			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	81
4			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	81
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	81



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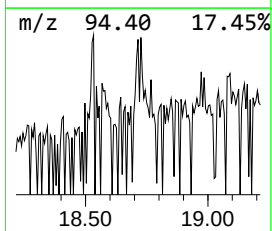
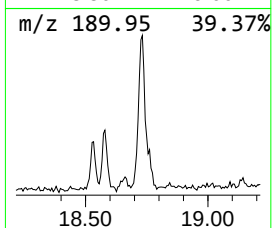
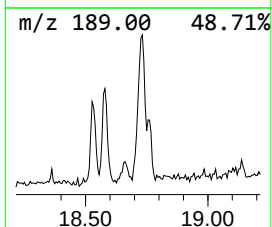
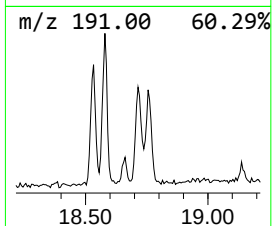
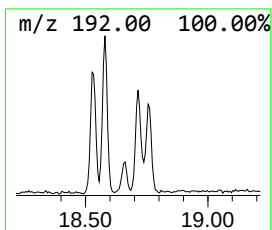
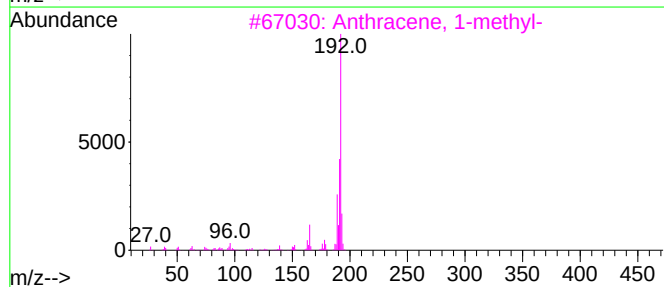
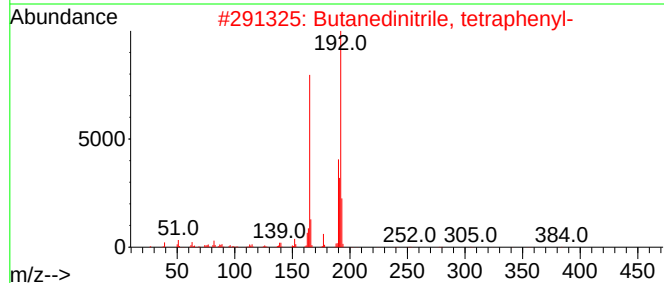
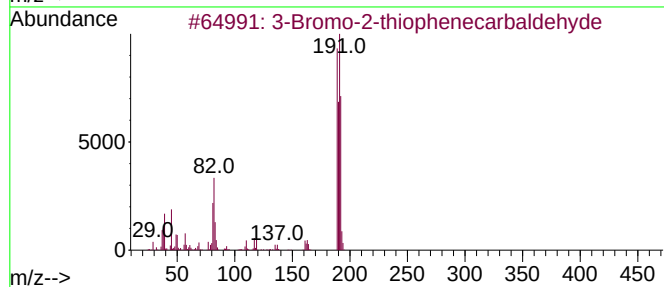
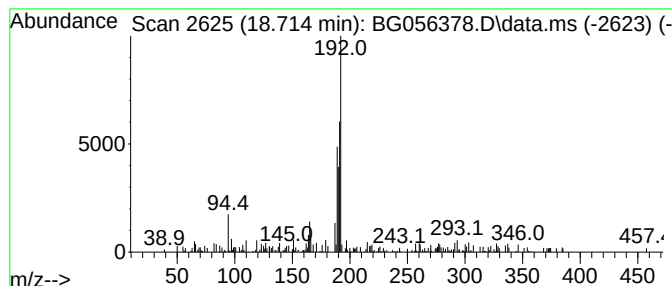
Instrument :
BNA_G
ClientSampleId :
OK-02-011923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3-Bromo-2-thiophenecarbalde... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.715	2.07 ng	66892	Phenanthrene-d10		17.663	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Bromo-2-thiophenecarbaldehyde		190	C5H3BrOS	000930-96-1	53
2	Butanedinitrile, tetraphenyl-		384	C28H20N2	003122-21-2	49
3	Anthracene, 1-methyl-		192	C15H12	000610-48-0	46
4	Naphtho[2,3-b]norbornadiene		192	C15H12	107426-38-0	46
5	1H-Indene, 2-phenyl-		192	C15H12	004505-48-0	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012023\
Data File : BG056378.D
Acq On : 20 Jan 2023 22:13
Operator : CG/JU
Sample : 01229-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-02-011923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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-...	5.348	14.1	ng	198156	1	8.309	281103	20.0
unknown9.414	9.414	3.1	ng	43246	1	8.309	281103	20.0
Benzophenone	16.259	7.3	ng	199197	3	14.925	545925	20.0
n-Hexadecanoic ...	18.509	3.8	ng	122692	4	17.663	647200	20.0
Anthracene, 2-m...	18.579	3.2	ng	104242	4	17.663	647200	20.0
3-Bromo-2-thiop...	18.715	2.1	ng	66892	4	17.663	647200	20.0