

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102021\
 Data File : BG050657.D
 Acq On : 20 Oct 2021 22:58
 Operator : CG/JU
 Sample : M4269-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RT-4197

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-BG100621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050657.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.788	384	391	406	rVB	739837	1270865	52.85%	4.689%
2	7.392	656	664	673	rBV	768320	1385136	57.60%	5.110%
3	8.249	803	810	821	rVB	194180	343866	14.30%	1.269%
4	9.424	1001	1010	1023	rVB	471486	895556	37.24%	3.304%
5	10.817	1240	1247	1256	rBV	162130	274999	11.44%	1.015%
6	11.075	1283	1291	1298	rBV	264019	484209	20.13%	1.786%
7	13.490	1694	1702	1710	rBV	1111438	1817588	75.58%	6.706%
8	13.655	1724	1730	1737	rBV10	18236	54275	2.26%	0.200%
9	14.289	1834	1838	1840	rBV2	60557	84904	3.53%	0.313%
10	14.319	1841	1843	1847	rVB	51222	62016	2.58%	0.229%
11	14.607	1886	1892	1897	rBV6	66016	158191	6.58%	0.584%
12	14.695	1903	1907	1912	rVB2	115741	179950	7.48%	0.664%
13	14.871	1932	1937	1943	rVB	372993	627896	26.11%	2.316%
14	14.936	1944	1948	1956	rBV5	101420	218862	9.10%	0.807%
15	15.353	2016	2019	2025	rBV3	86414	129836	5.40%	0.479%
16	15.647	2066	2069	2076	rVB	160432	237316	9.87%	0.876%
17	16.087	2140	2144	2154	rVB	371350	598437	24.88%	2.208%
18	16.358	2185	2190	2199	rBV	695371	1190465	49.50%	4.392%
19	16.569	2221	2226	2231	rBV	1184497	1728980	71.90%	6.379%
20	17.392	2361	2366	2371	rBV	1569798	2404815	100.00%	8.872%
21	17.662	2409	2412	2418	rVB	890488	1196266	49.74%	4.413%
22	18.003	2467	2470	2475	rVB2	400308	553209	23.00%	2.041%
23	19.660	2748	2752	2758	rVB	1440079	2142962	89.11%	7.906%
24	20.024	2810	2814	2821	rVB	1115146	1702120	70.78%	6.280%
25	20.206	2841	2845	2850	rVB	1696612	2299817	95.63%	8.485%
26	21.904	3128	3134	3141	rBV3	531197	1453389	60.44%	5.362%
27	21.969	3141	3145	3153	rVB	466794	818329	34.03%	3.019%
28	24.242	3525	3532	3540	rBV	302203	976668	40.61%	3.603%
29	25.012	3658	3663	3675	rVB	199871	550446	22.89%	2.031%
30	25.171	3683	3690	3701	rVB	249553	744876	30.97%	2.748%
31	25.335	3711	3718	3726	rVB3	194976	519161	21.59%	1.915%

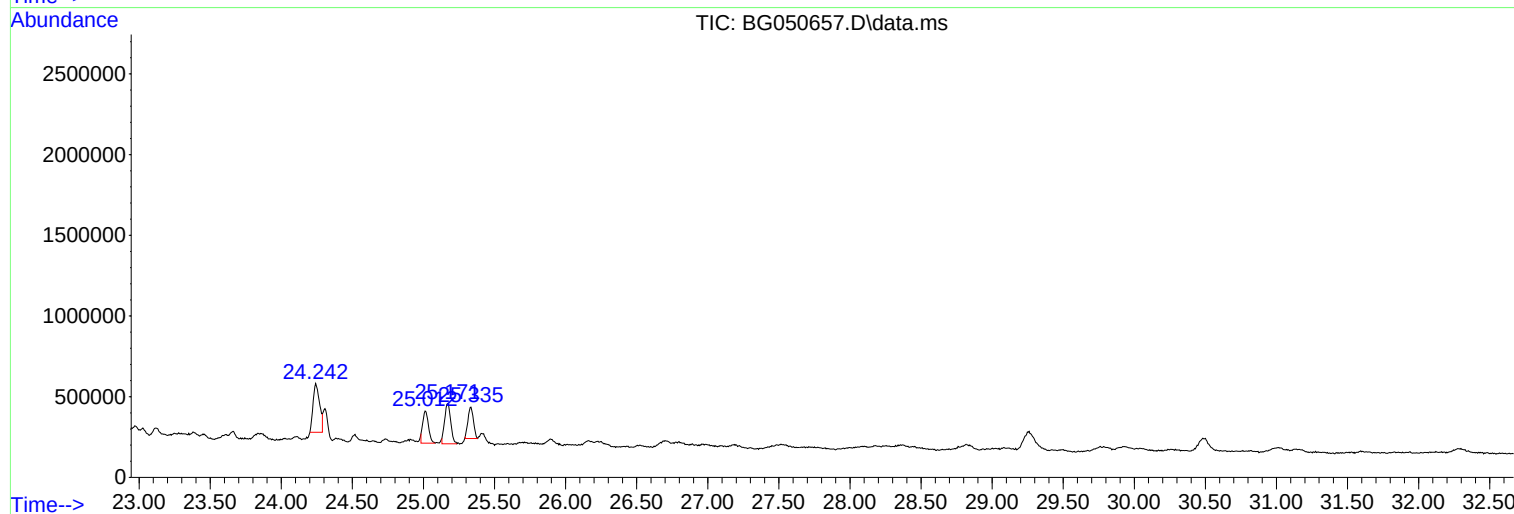
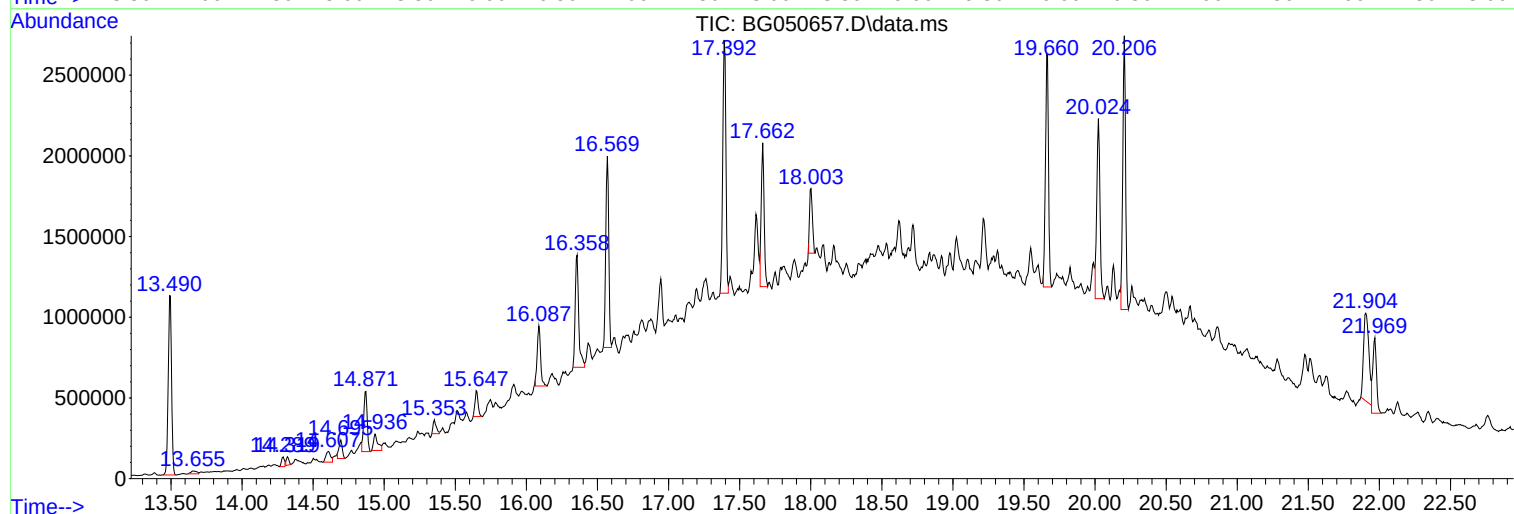
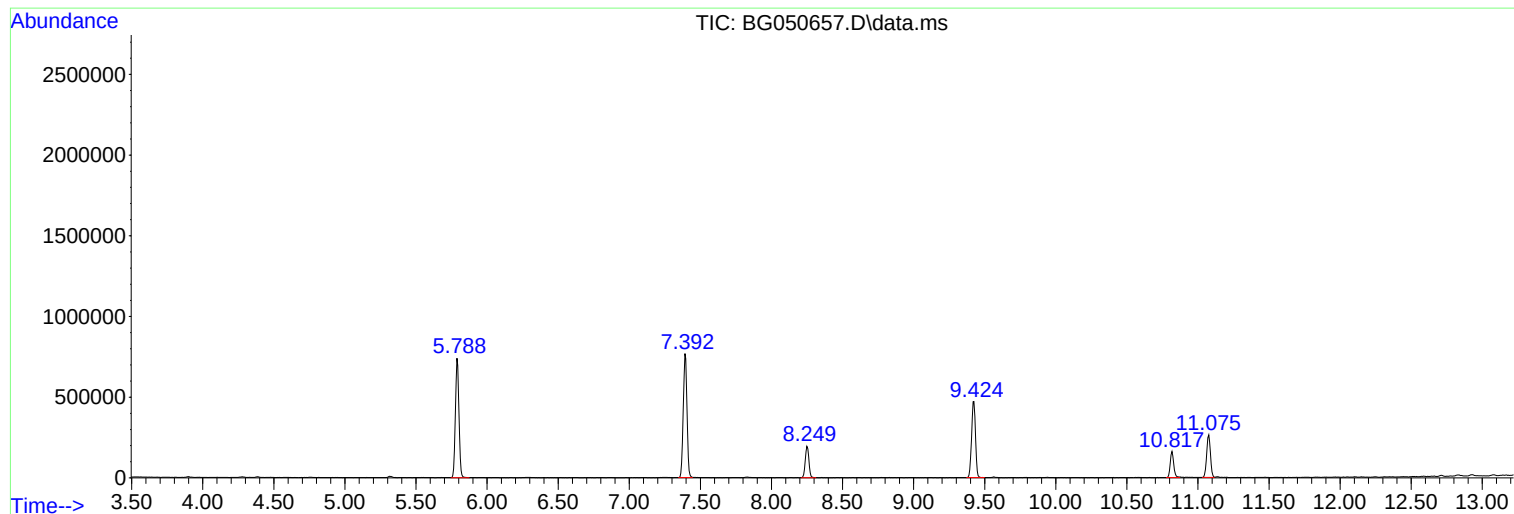
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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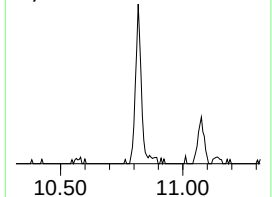
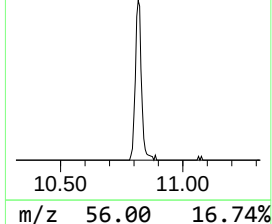
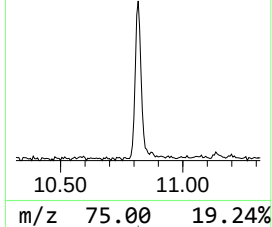
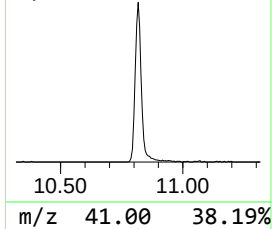
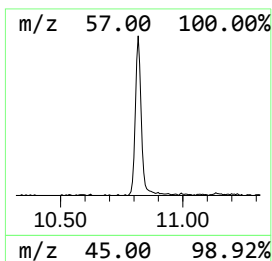
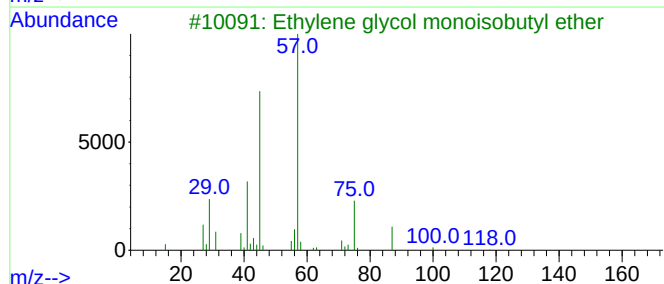
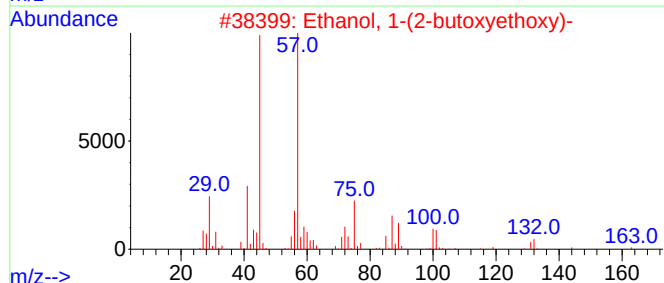
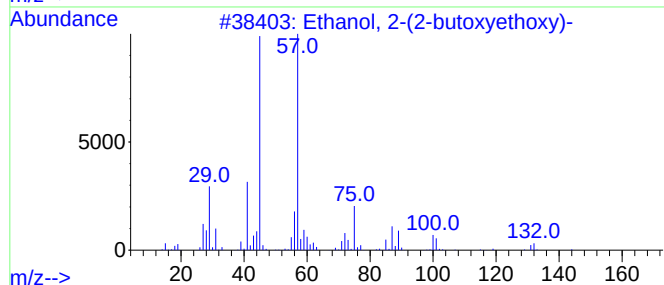
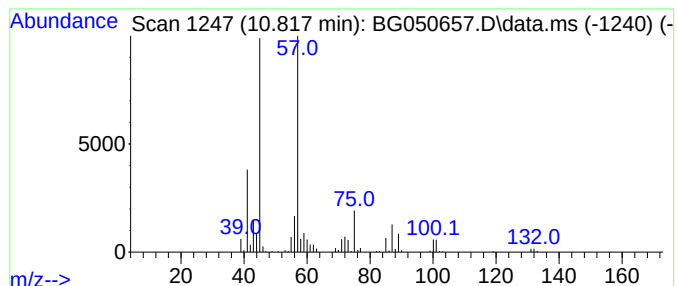
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.817	11.36 ng	274999	Naphthalene-d8	11.076

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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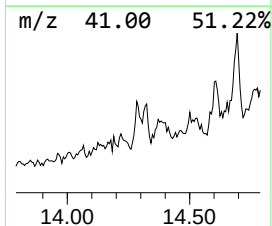
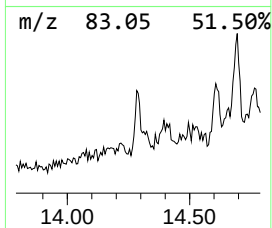
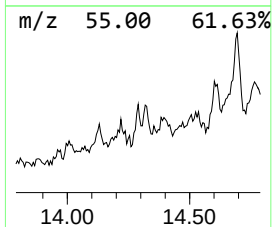
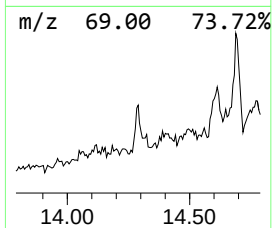
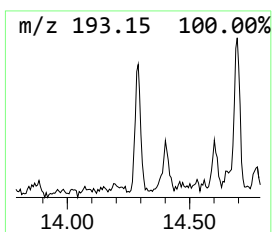
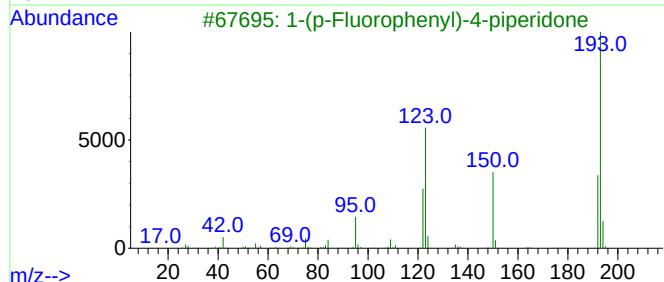
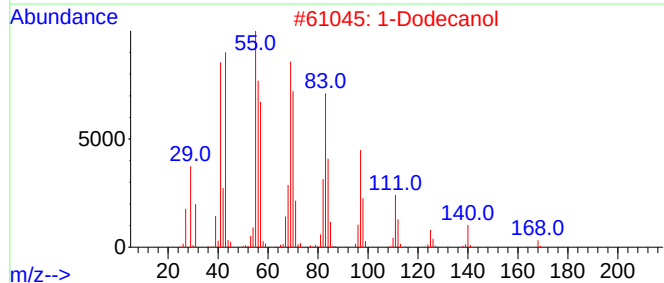
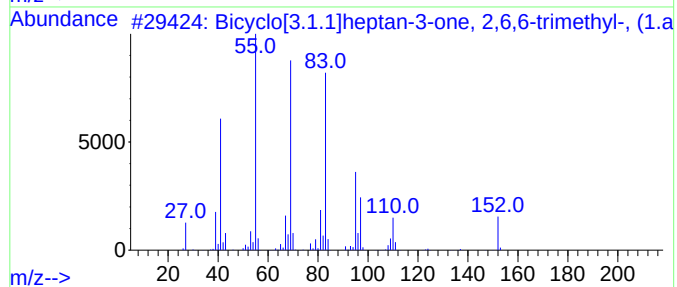
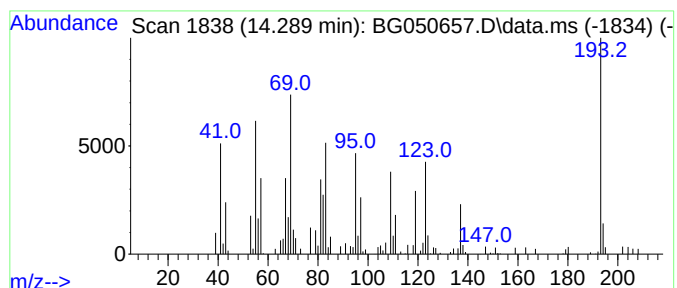
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown14.289 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.289	2.70 ng	84904	Acenaphthene-d10	14.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	27
2			1-Dodecanol	186	C12H26O	000112-53-8	25
3			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	25
4			Neopentylidenecyclohexane	152	C11H20	039546-80-0	22
5			Octanenitrile	125	C8H15N	000124-12-9	22



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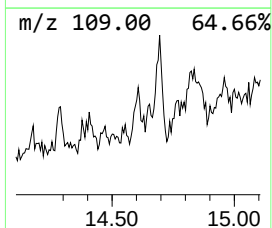
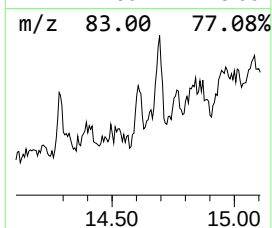
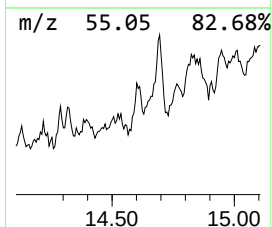
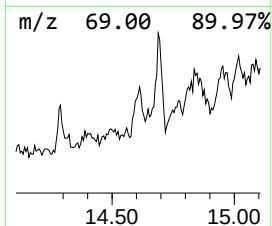
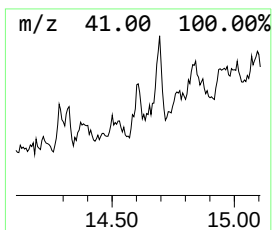
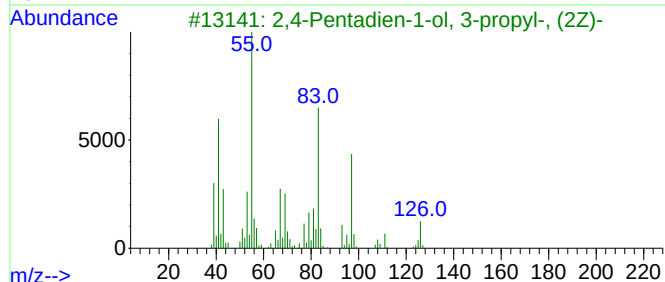
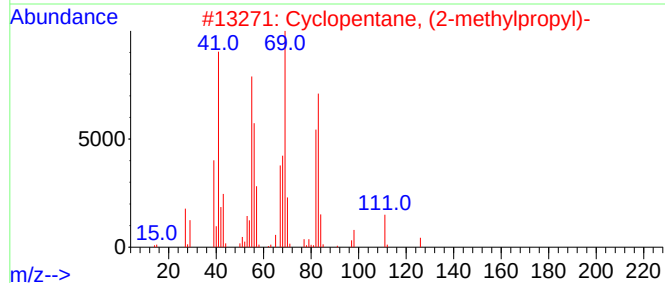
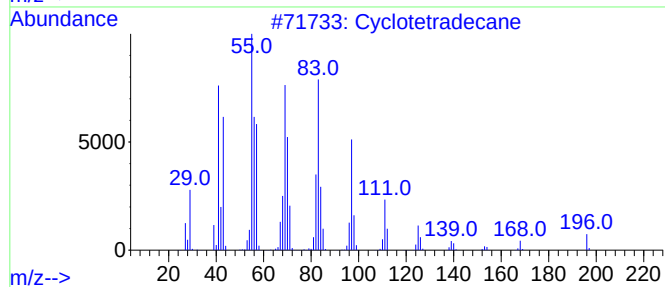
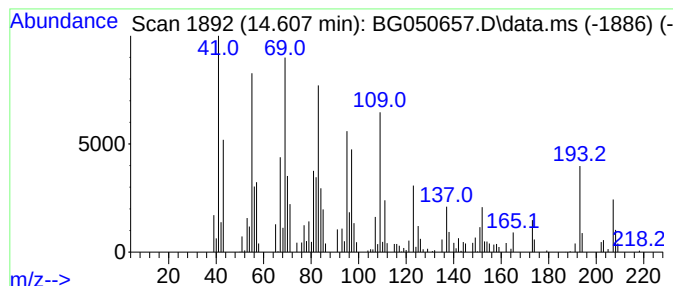
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown14.607 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.607	5.04 ng	158191	Acenaphthene-d10	14.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	43
2			Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	30
3			2,4-Pentadien-1-ol, 3-propyl-, (...)	126	C8H14O	1000142-17-9	20
4			1-Hexadecanol	242	C16H34O	036653-82-4	20
5			1,1'-Bicyclohexyl, 2-ethyl-, cis-	194	C14H26	050991-12-3	20



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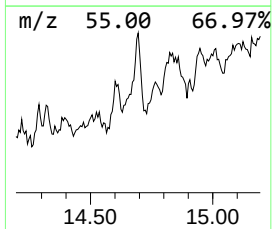
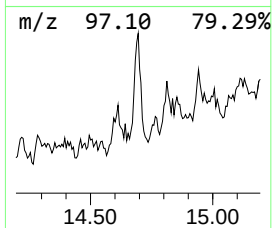
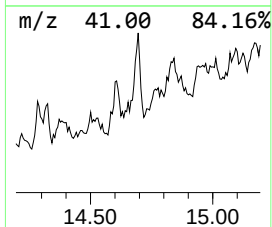
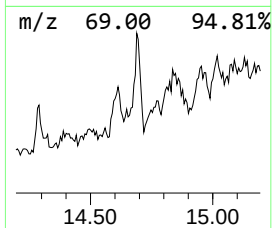
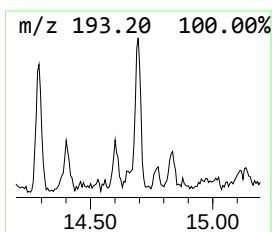
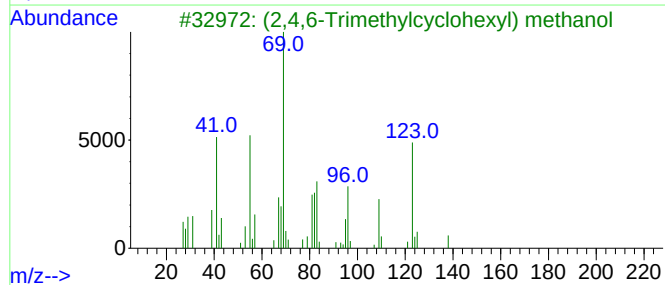
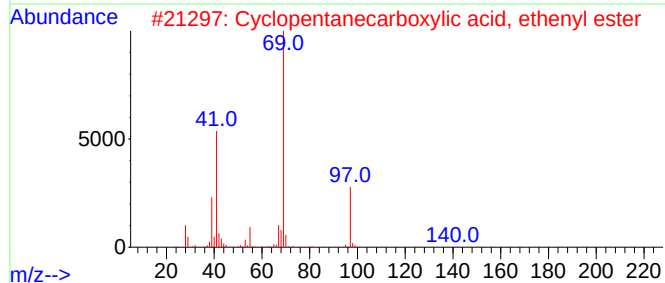
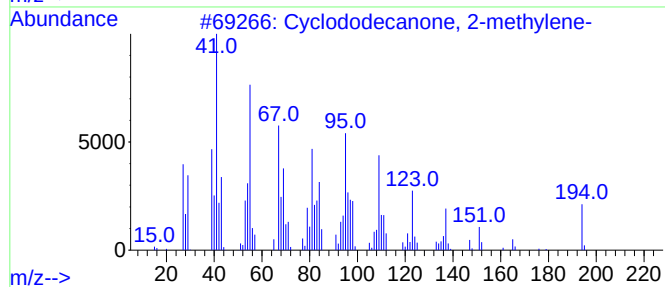
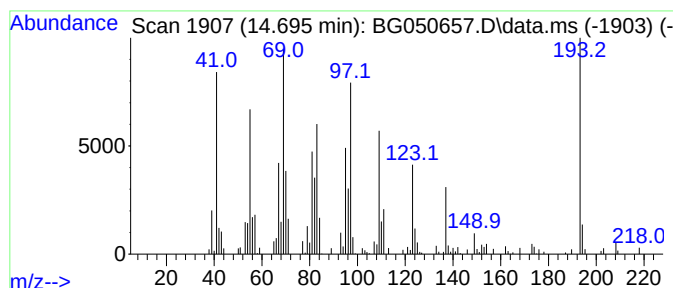
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.695 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.695	5.73 ng	179950	Acenaphthene-d10	14.871	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	38
2	Cyclopentanecarboxylic acid, eth...	140	C8H12O2	016523-06-1	22
3	(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	22
4	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054824-04-3	18
5	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	18



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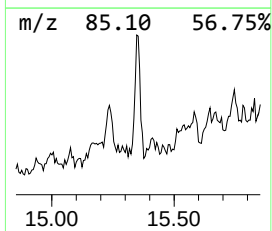
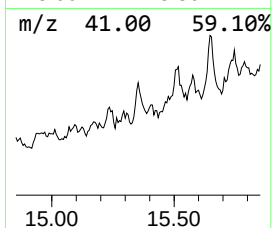
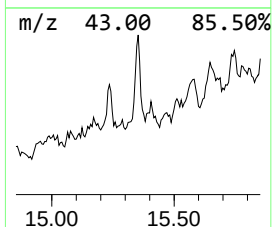
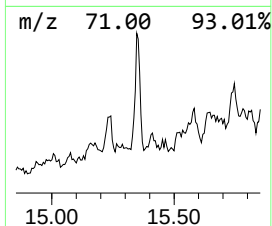
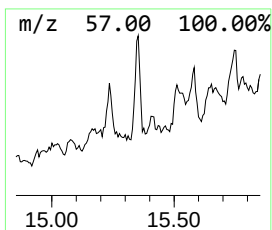
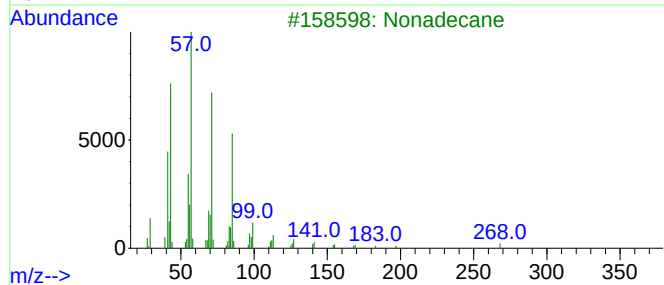
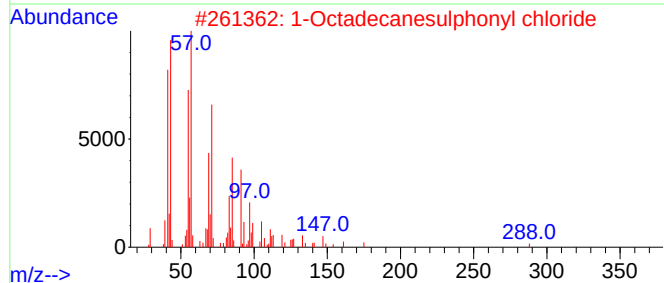
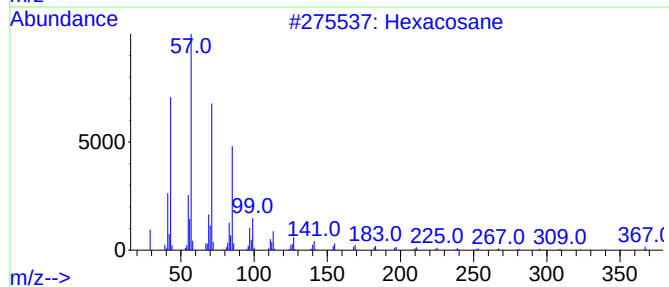
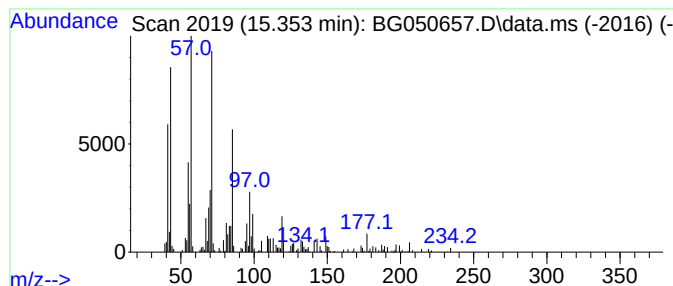
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.353	4.14 ng	129836	Acenaphthene-d10	14.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	72
2			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	72
3			Nonadecane	268	C19H40	000629-92-5	64
4			Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	59
5			Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	59



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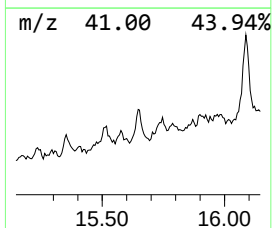
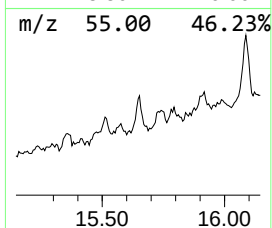
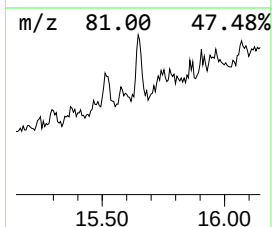
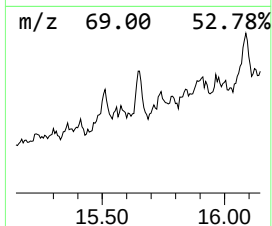
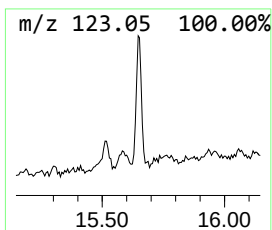
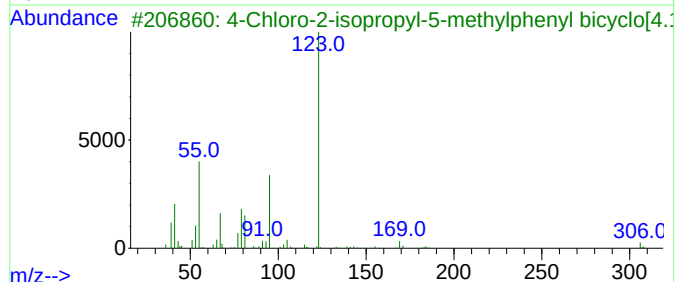
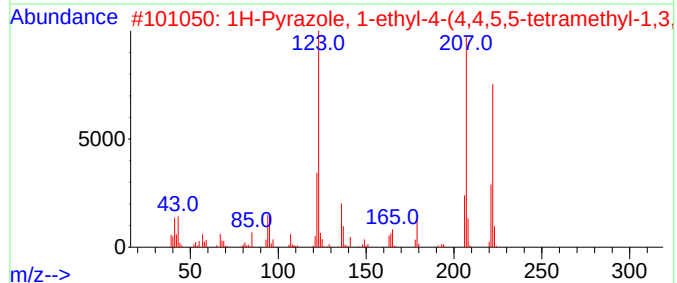
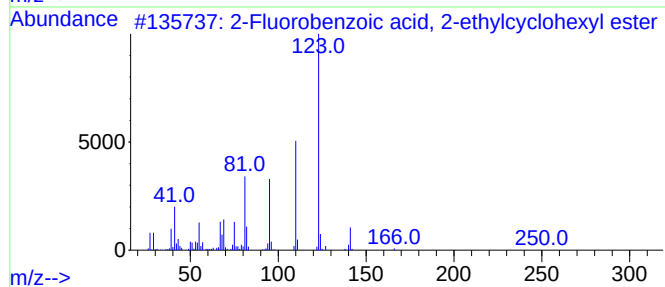
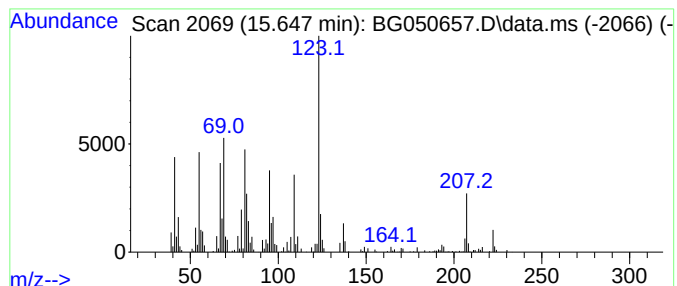
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Fluorobenzoic acid, 2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	7.56 ng	237316	Acenaphthene-d10	14.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19F02	1000278-98-1	50
2			1H-Pyrazole, 1-ethyl-4-(4,4,5,5-...	222	C11H19BN2O2	1010319-69-6	47
3			4-Chloro-2-isopropyl-5-methylphe...	306	C18H23ClO2	321918-37-0	43
4			N-[(2-Fluorophenyl)carbonyl]glycine	197	C9H8FN03	000363-34-8	43
5			Phorone	138	C9H14O	000504-20-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102021\
Data File : BG050657.D
Acq On : 20 Oct 2021 22:58
Operator : CG/JU
Sample : M4269-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-4197

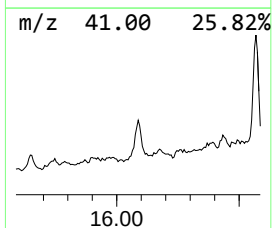
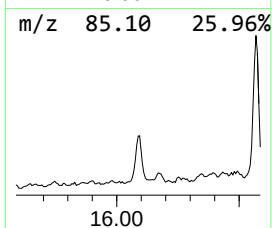
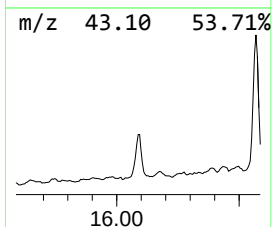
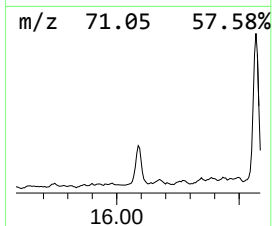
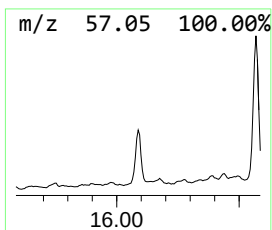
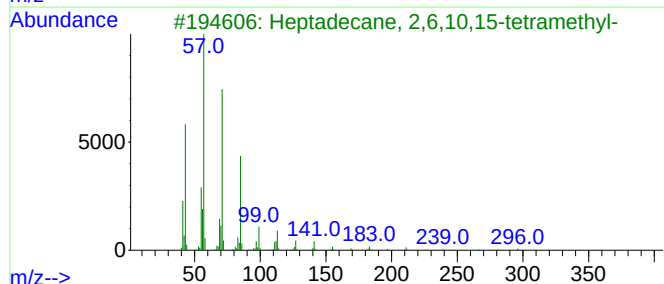
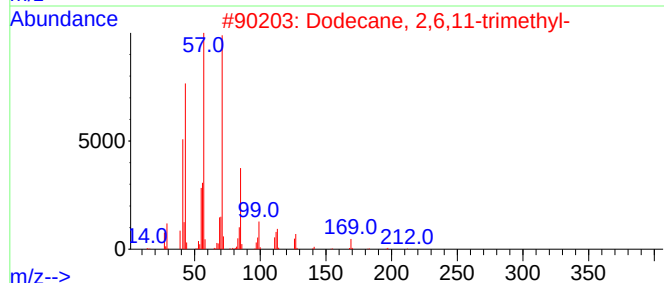
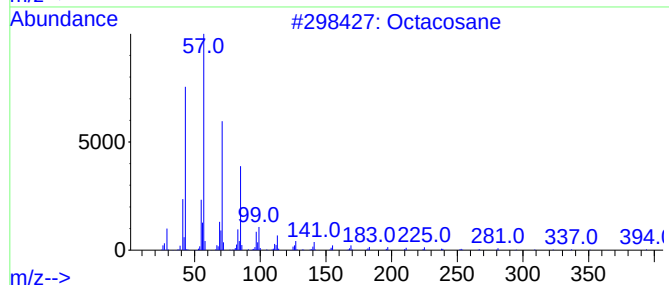
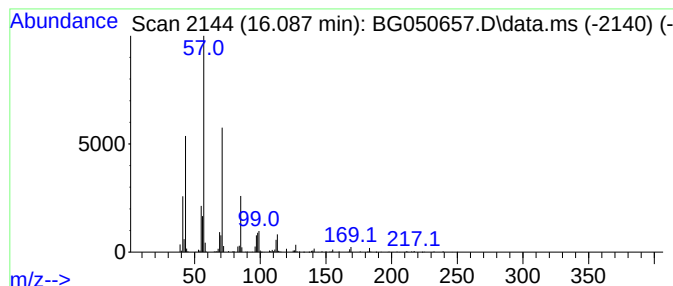
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.087	19.06 ng	598437	Acenaphthene-d10	14.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	83
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4			Hexadecane	226	C16H34	000544-76-3	78
5			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102021\
Data File : BG050657.D
Acq On : 20 Oct 2021 22:58
Operator : CG/JU
Sample : M4269-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

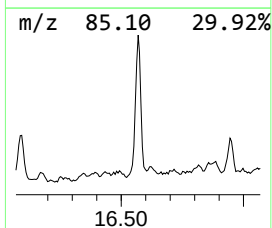
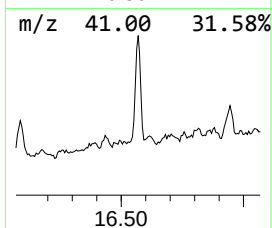
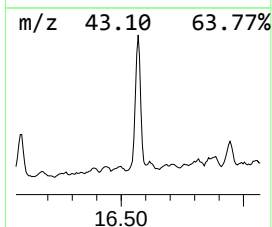
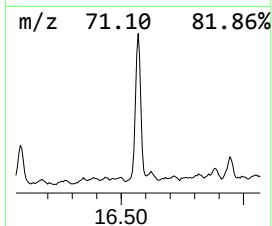
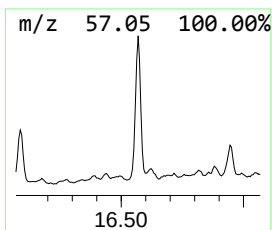
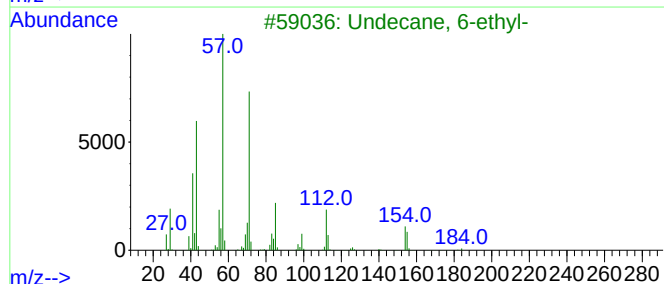
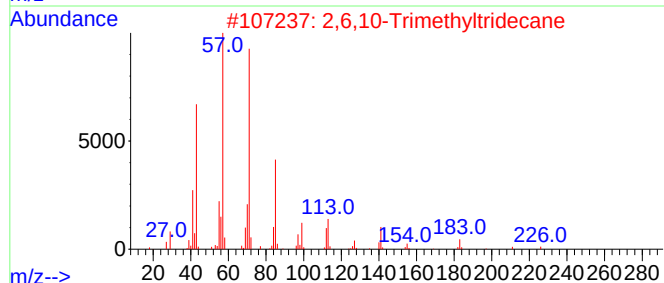
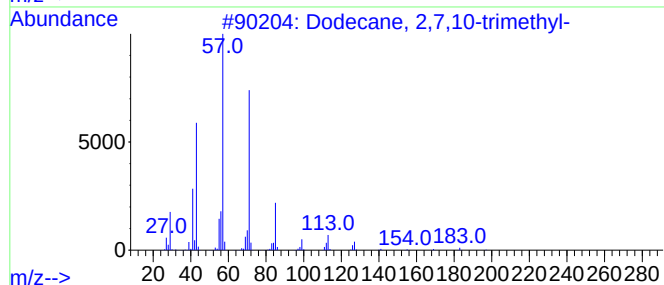
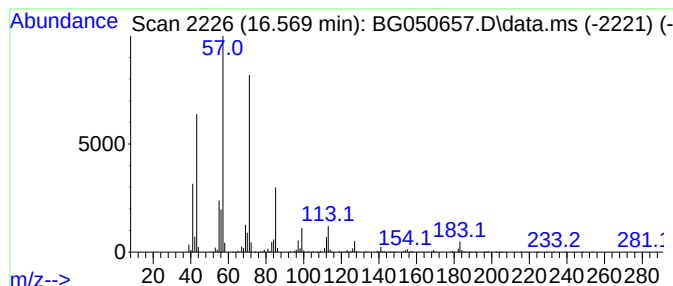
Instrument :
BNA_G
ClientSampleId :
RT-4197

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dodecane, 2,7,10-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.569	28.91 ng	1728980	Phenanthrene-d10		17.615	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-		212	C15H32	074645-98-0	90
2	2,6,10-Trimethyltridecane		226	C16H34	003891-99-4	90
3	Undecane, 6-ethyl-		184	C13H28	017312-60-6	87
4	Tridecane, 5-propyl-		226	C16H34	055045-11-9	86
5	Heptane, 2,6-dimethyl-		128	C9H20	001072-05-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102021\
Data File : BG050657.D
Acq On : 20 Oct 2021 22:58
Operator : CG/JU
Sample : M4269-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

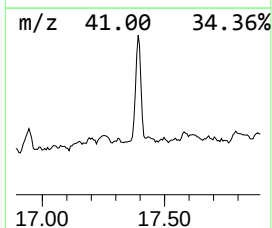
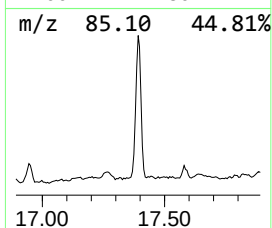
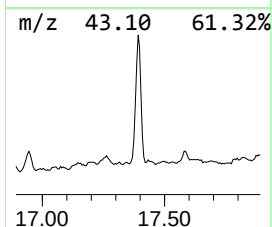
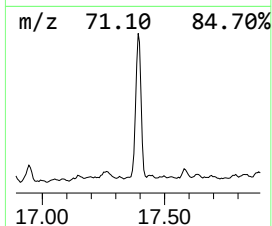
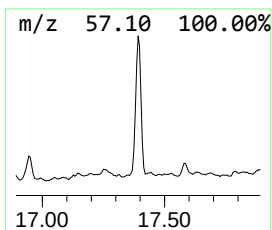
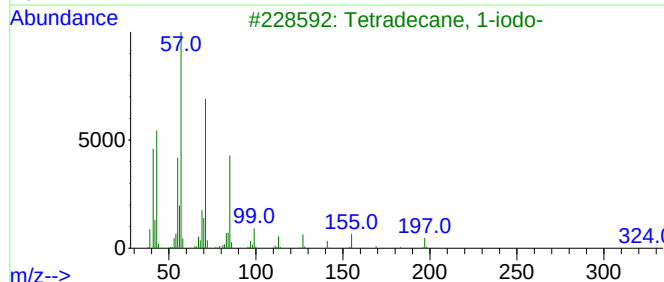
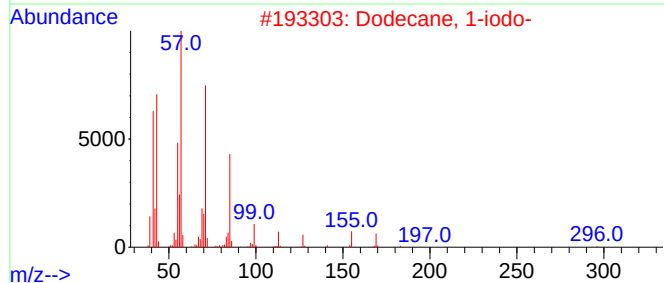
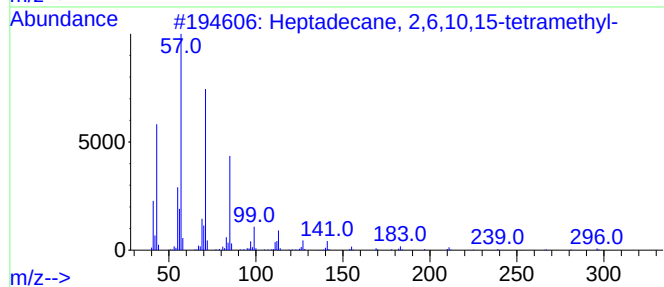
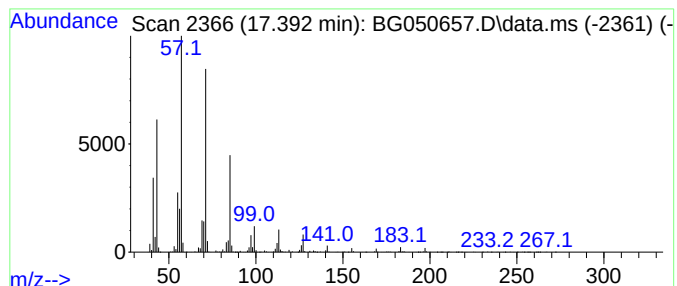
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 2,6,10,15-tetr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.392	40.21 ng	2404820	Phenanthrene-d10		17.615	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	91
2	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	90
3	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	90
4	Hexadecane, 4-methyl-		240	C17H36	025117-26-4	83
5	Heptacosane		380	C27H56	000593-49-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102021\
Data File : BG050657.D
Acq On : 20 Oct 2021 22:58
Operator : CG/JU
Sample : M4269-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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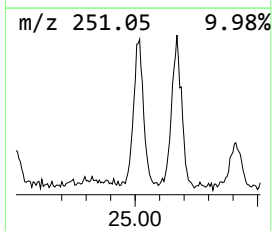
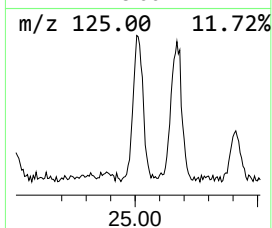
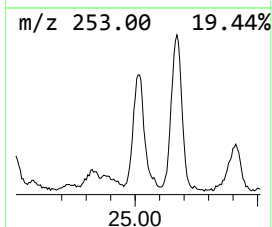
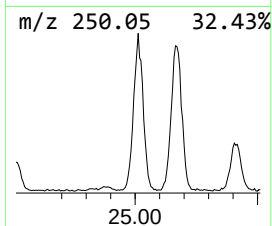
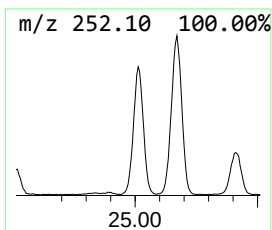
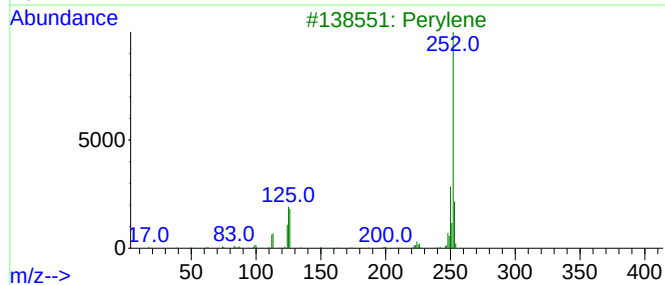
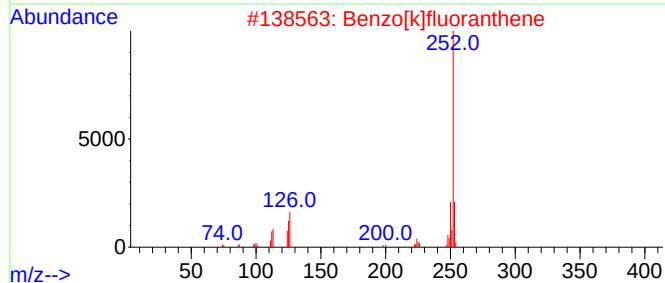
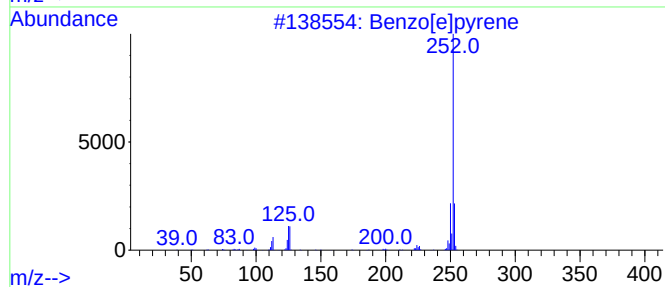
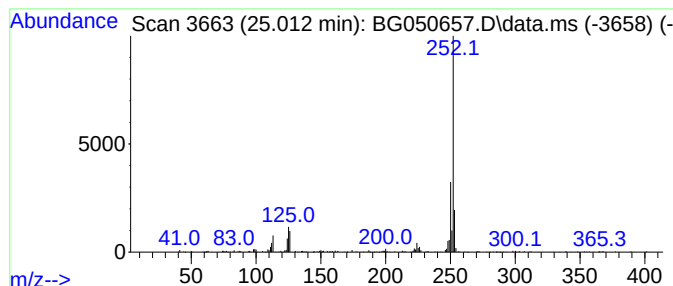
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.012	21.21 ng	550446	Perylene-d12	25.335

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3			Perylene	252	C20H12	000198-55-0	96
4			Benzo[a]pyrene	252	C20H12	000050-32-8	94
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102021\
Data File : BG050657.D
Acq On : 20 Oct 2021 22:58
Operator : CG/JU
Sample : M4269-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RT-4197

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.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
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unknown14.289	14.289	2.7	ng	84904	3	14.871	627896	20.0
unknown14.607	14.607	5.0	ng	158191	3	14.871	627896	20.0
unknown14.695	14.695	5.7	ng	179950	3	14.871	627896	20.0
Hexacosane	15.353	4.1	ng	129836	3	14.871	627896	20.0
2-Fluorobenzoic...	15.647	7.6	ng	237316	3	14.871	627896	20.0
Octacosane	16.087	19.1	ng	598437	3	14.871	627896	20.0
Dodecane, 2,7,1...	16.569	28.9	ng	1728980	4	17.615	1196270	20.0
Heptadecane, 2,...	17.392	40.2	ng	2404820	4	17.615	1196270	20.0
Benzo[e]pyrene	25.012	21.2	ng	550446	6	25.335	519161	20.0