

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042121\
 Data File : BG048830.D
 Acq On : 21 Apr 2021 22:07
 Operator : CG/JU
 Sample : M1998-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-4A

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-BG041421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048830.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.130	298	305	313	rVB	85386	130533	11.82%	1.942%
2	5.612	375	387	395	rBV	247955	393633	35.65%	5.857%
3	7.228	653	662	665	rBV	364589	723743	65.55%	10.769%
4	8.062	797	804	809	rBV2	98422	165903	15.03%	2.469%
5	8.115	809	813	818	rVB3	10050	16844	1.53%	0.251%
6	9.231	995	1003	1014	rBV	237333	422882	38.30%	6.292%
7	10.588	1230	1234	1242	rBV4	12482	28541	2.59%	0.425%
8	10.888	1276	1285	1291	rBV2	134777	238947	21.64%	3.555%
9	12.380	1532	1539	1547	rVB	71555	123979	11.23%	1.845%
10	13.338	1695	1702	1709	rBV	590461	869809	78.78%	12.942%
11	14.161	1836	1842	1848	rVB2	16676	32492	2.94%	0.483%
12	14.454	1885	1892	1894	rBV3	6889	13092	1.19%	0.195%
13	14.719	1929	1937	1943	rVB	205819	323029	29.26%	4.806%
14	16.217	2186	2192	2201	rBV	82329	127695	11.57%	1.900%
15	16.987	2319	2323	2329	rBV5	6872	15274	1.38%	0.227%
16	17.480	2399	2407	2412	rBV	253723	388535	35.19%	5.781%
17	17.521	2412	2414	2416	rVV2	27035	33670	3.05%	0.501%
18	17.551	2416	2419	2422	rVV	38327	49438	4.48%	0.736%
19	17.592	2422	2426	2433	rVB5	14602	33817	3.06%	0.503%
20	18.514	2580	2583	2587	rBV3	16564	22503	2.04%	0.335%
21	19.090	2677	2681	2685	rBV7	10209	15876	1.44%	0.236%
22	19.272	2708	2712	2715	rBV6	18634	27097	2.45%	0.403%
23	19.366	2724	2728	2732	rBV	52425	64361	5.83%	0.958%
24	19.537	2752	2757	2761	rBV2	60793	90942	8.24%	1.353%
25	19.901	2815	2819	2825	rVB2	63110	89626	8.12%	1.334%
26	19.972	2827	2831	2834	rBV6	9903	15509	1.40%	0.231%
27	20.089	2846	2851	2857	rVB	865382	1104047	100.00%	16.427%
28	20.383	2898	2901	2906	rVB7	21760	37495	3.40%	0.558%
29	20.923	2991	2993	2994	rBV2	12485	11647	1.05%	0.173%
30	21.346	3061	3065	3068	rBV6	13710	22584	2.05%	0.336%
31	21.393	3069	3073	3078	rVV2	73806	101511	9.19%	1.510%
32	21.646	3112	3116	3121	rVB3	40376	60717	5.50%	0.903%
33	21.775	3132	3138	3144	rBV	226057	401624	36.38%	5.976%
34	24.037	3518	3523	3526	rBV6	22443	43066	3.90%	0.641%
35	24.196	3545	3550	3552	rBV5	9700	18950	1.72%	0.282%
36	24.789	3646	3651	3652	rBV5	20623	29237	2.65%	0.435%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	24.942	3669	3677	3679	rBV6	24005	52892	4.79%	0.787%
38	25.107	3696	3705	3715	rBV2	130522	379204	34.35%	5.642%

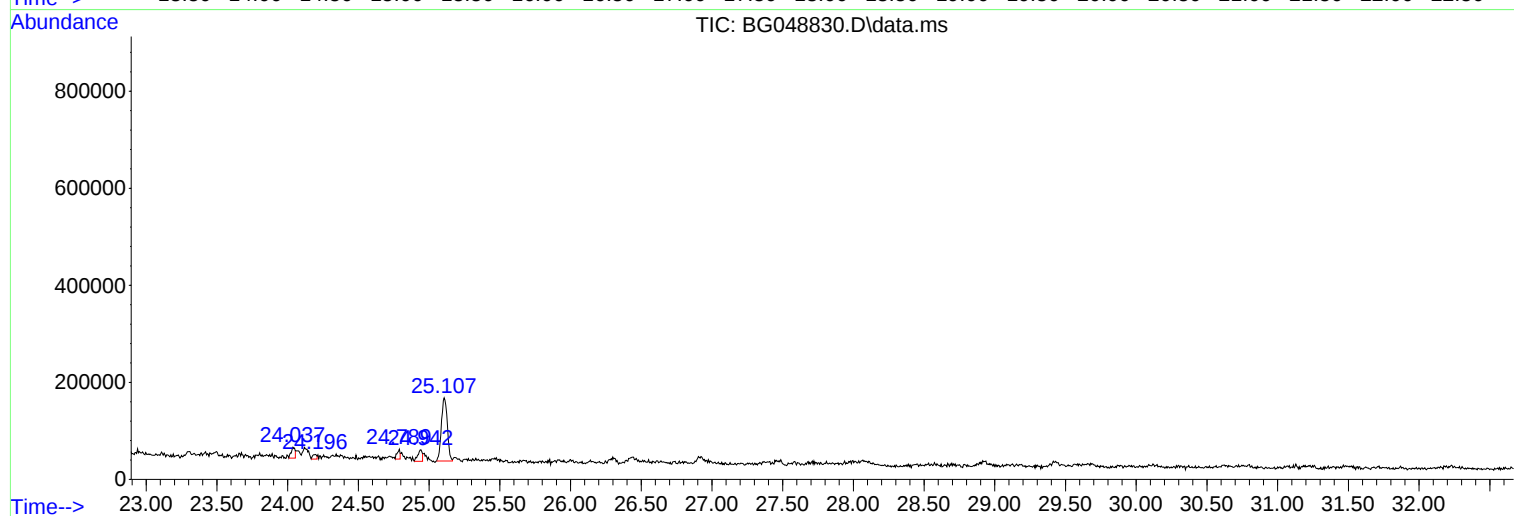
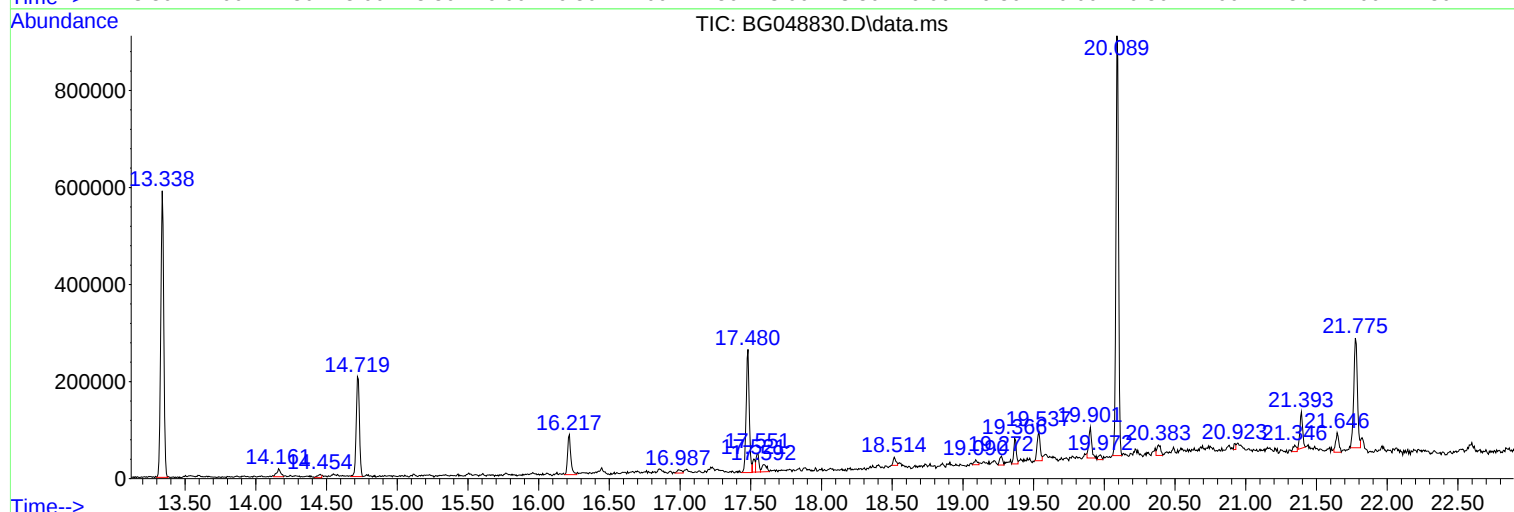
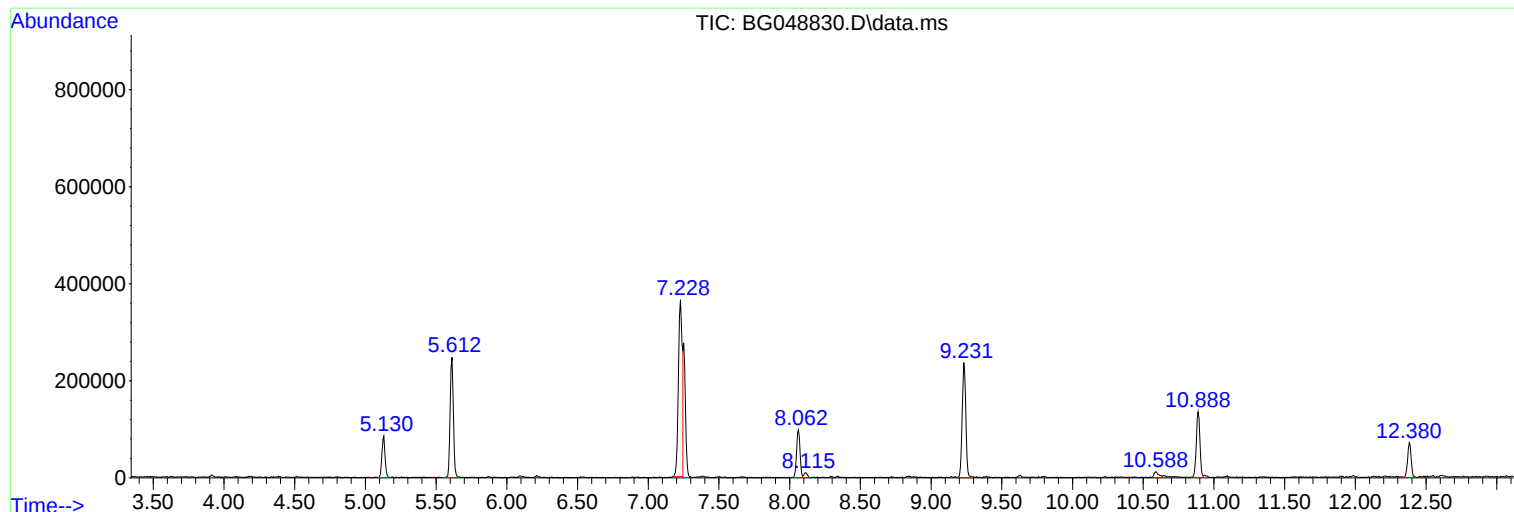
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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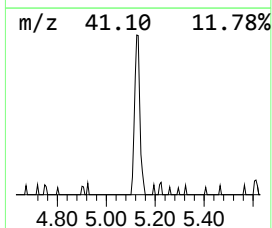
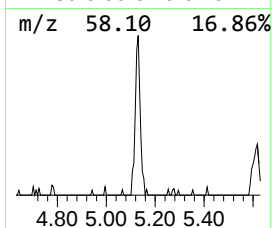
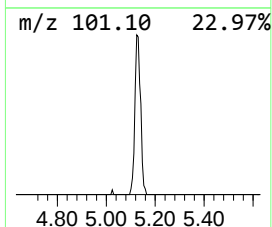
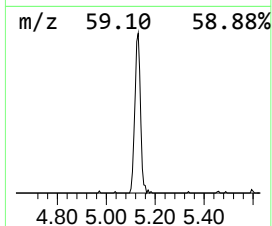
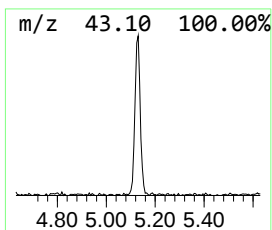
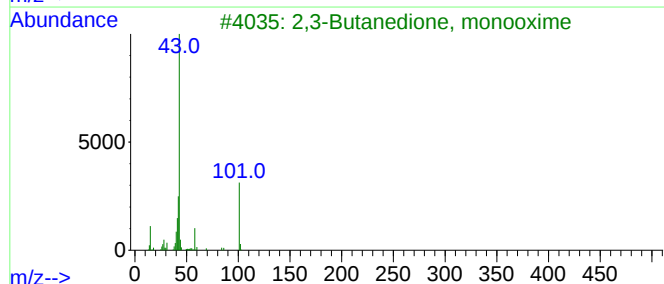
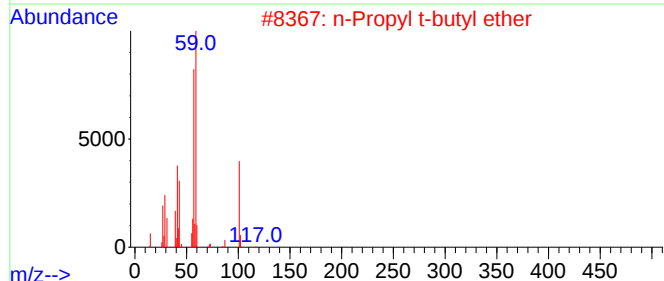
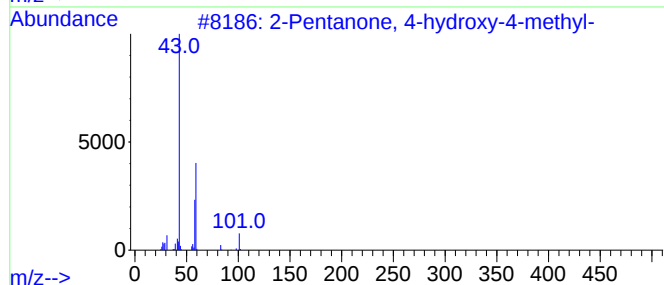
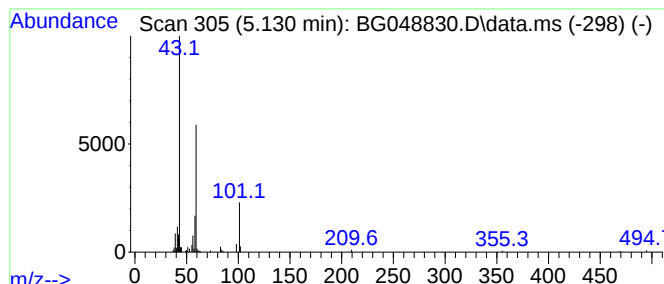
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.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.
5.130	15.74 ng	130533	1,4-Dichlorobenzene-d4	8.056

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39		
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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Misc :
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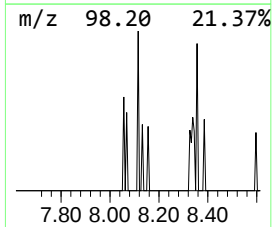
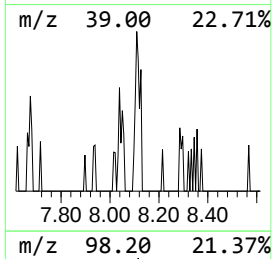
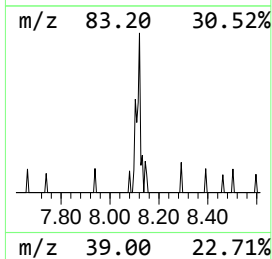
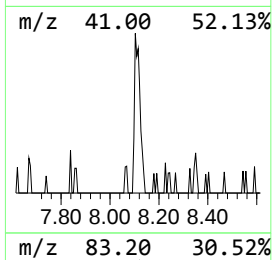
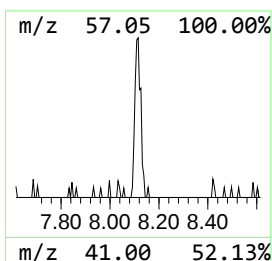
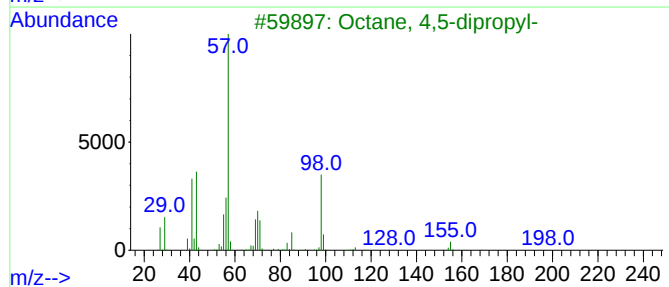
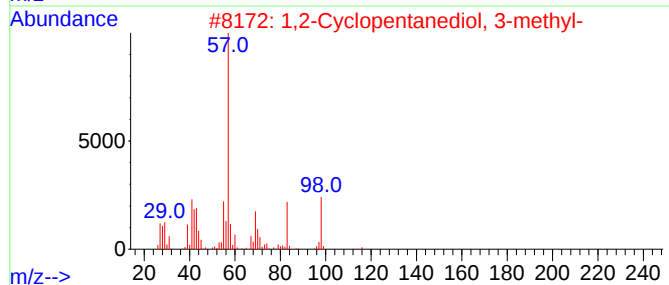
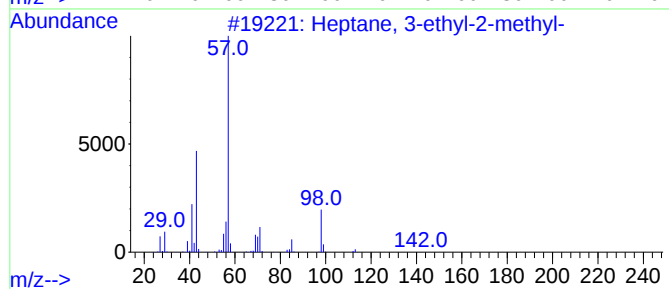
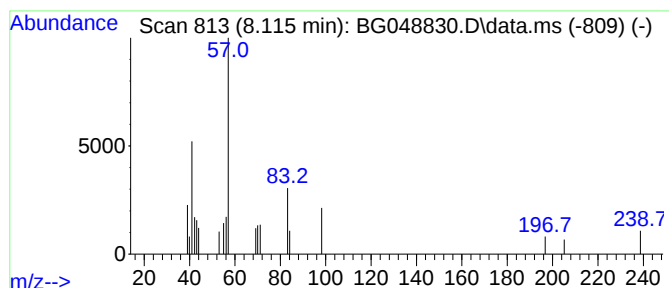
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown8.115 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.115	2.03 ng	16844	1,4-Dichlorobenzene-d4	8.056

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	47
2			1,2-Cyclopentanediol, 3-methyl-	116	C6H12O2	027583-37-5	47
3			Octane, 4,5-dipropyl-	198	C14H30	020905-05-9	47
4			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	37
5			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	1000365-19-6	32



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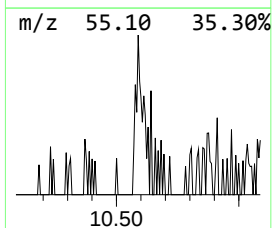
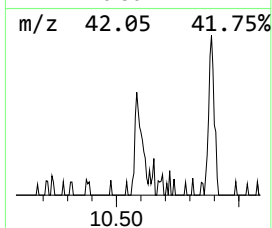
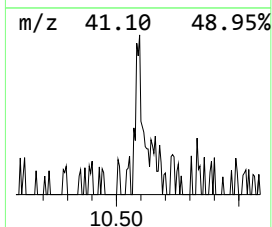
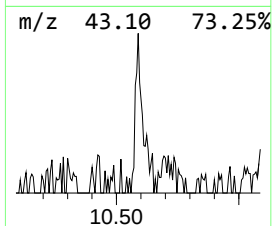
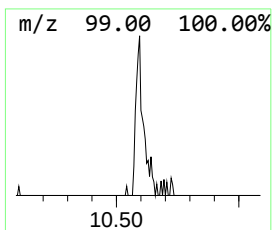
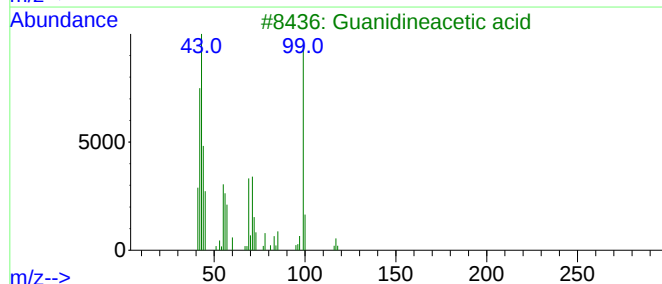
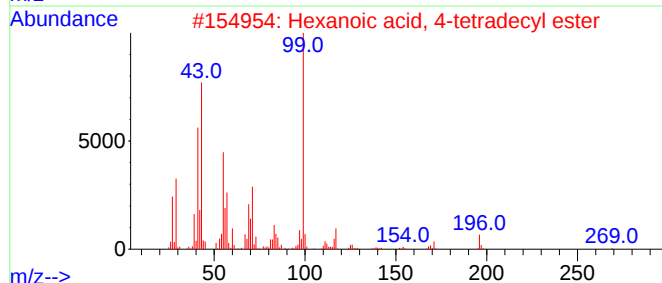
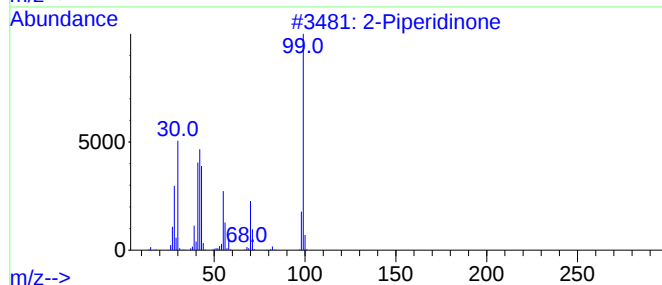
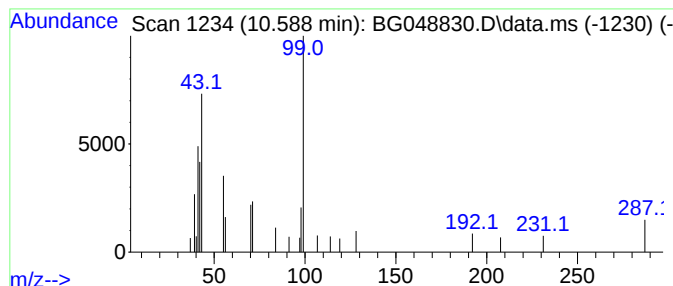
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Piperidinone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.588	2.39 ng	28541	Naphthalene-d8	10.888

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Piperidinone	99	C5H9NO	000675-20-7	64
2			Hexanoic acid, 4-tetradecyl ester	312	C20H40O2	1000279-29-8	47
3			Guanidineacetic acid	117	C3H7N3O2	000352-97-6	47
4			2H-Pyran-2-one, 6-heptyltetrahydro-	198	C12H22O2	000713-95-1	47
5			trans-4-Hydroxy-3-methylundecano...	198	C12H22O2	148806-10-4	42



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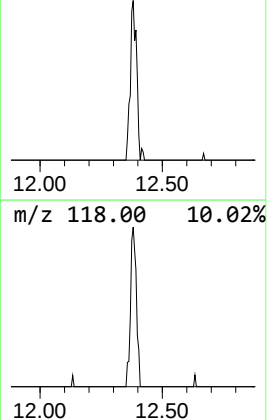
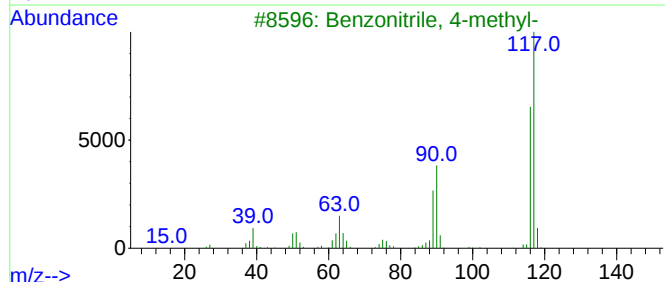
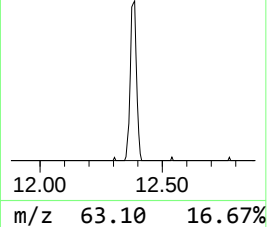
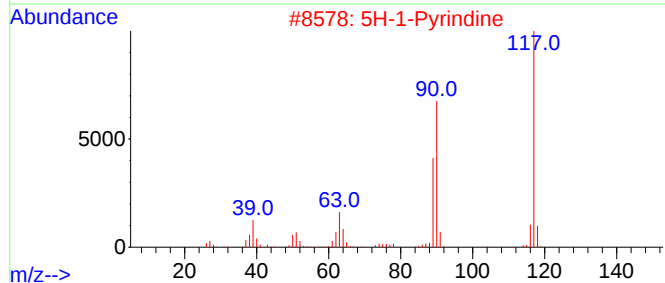
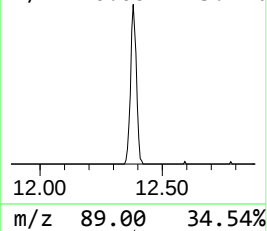
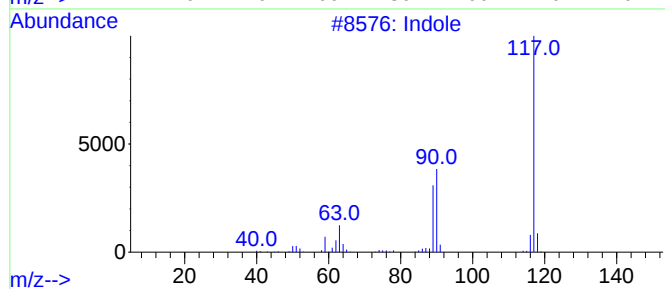
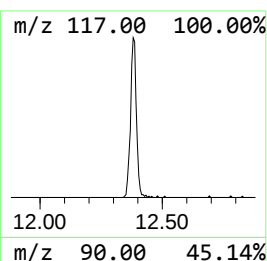
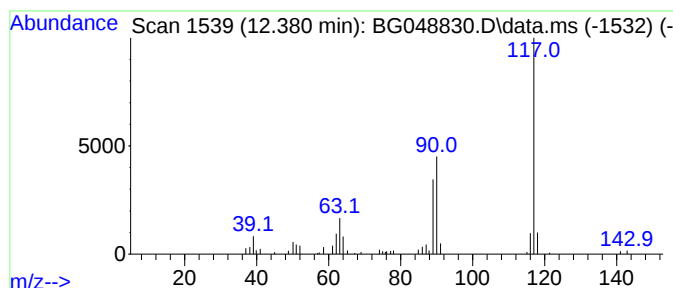
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 4 Indole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.380	10.38 ng	123979	Naphthalene-d8	10.888

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	94
2			5H-1-Pyridine	117	C8H7N	000270-91-7	91
3			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	91
4			Indolizine	117	C8H7N	000274-40-8	91
5			Benzyl nitrile	117	C8H7N	000140-29-4	91



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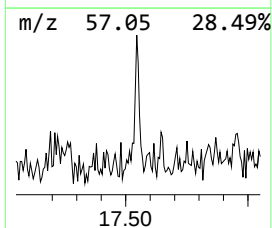
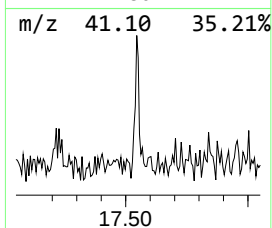
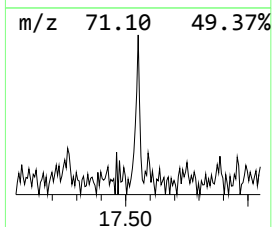
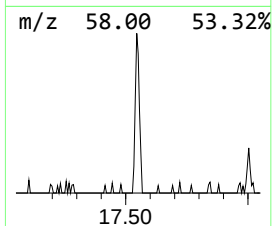
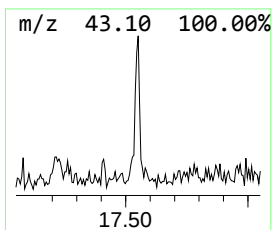
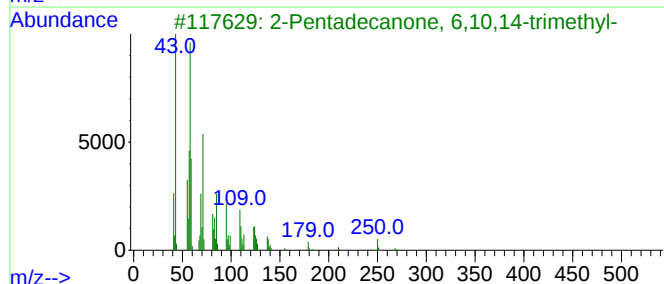
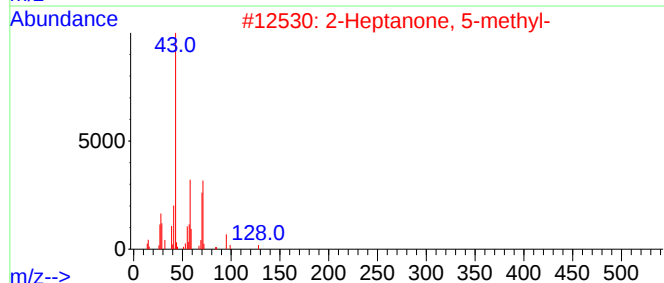
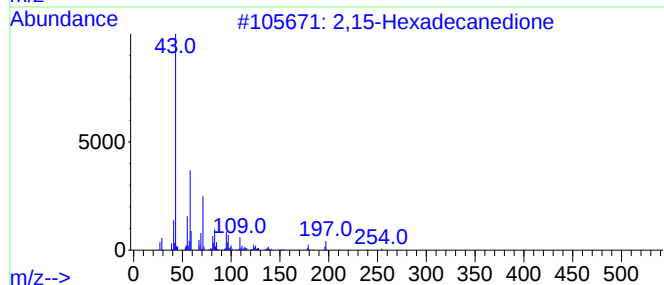
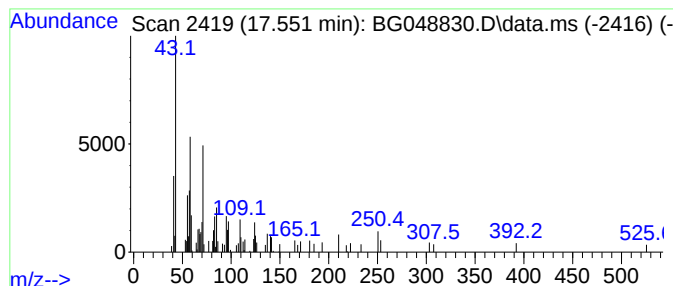
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown17.551 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.551	2.54 ng	49438	Phenanthrene-d10	17.480

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,15-Hexadecanedione	254	C16H30O2	018650-13-0	47	
2	2-Heptanone, 5-methyl-	128	C8H16O	018217-12-4	43	
3	2-Pentadecanone, 6,10,14-trimethyl-	268	C18H36O	000502-69-2	32	
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	27	
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	27	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042121\
Data File : BG048830.D
Acq On : 21 Apr 2021 22:07
Operator : CG/JU
Sample : M1998-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-4A

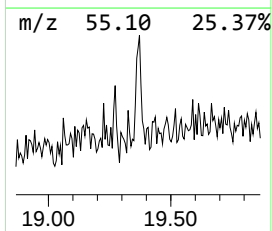
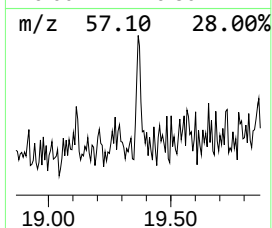
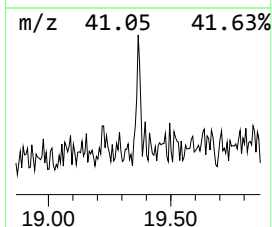
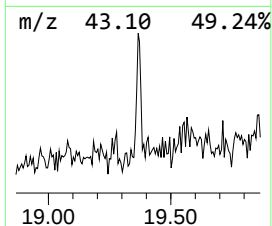
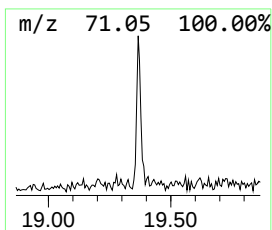
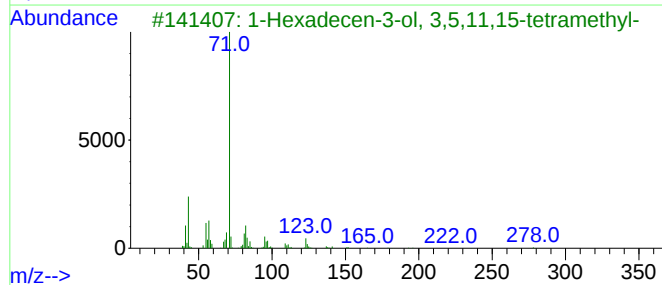
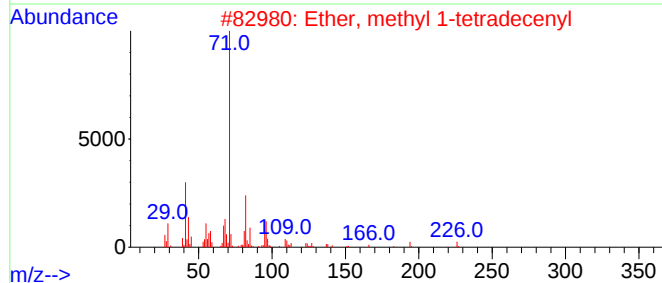
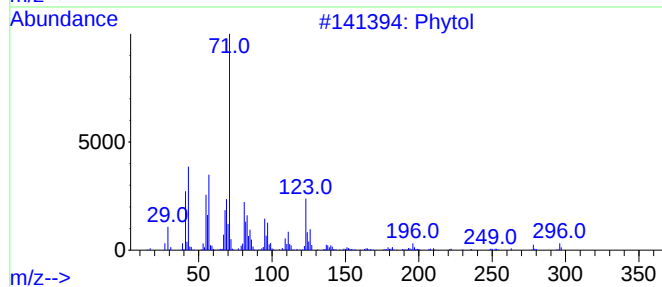
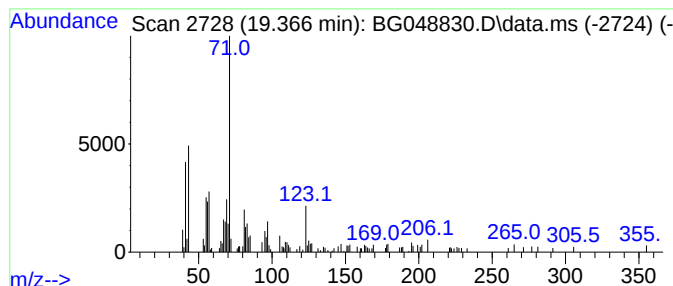
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Phytol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.366	3.31 ng	64361	Phenanthrene-d10	17.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phytol			296	C20H40O	000150-86-7	53
2	Ether, methyl 1-tetradecenyl			226	C15H30O	026537-05-3	49
3	1-Hexadecen-3-ol, 3,5,11,15-tetr...			296	C20H40O	1000262-55-5	47
4	Ether, 1-hexadecenyl methyl			254	C17H34O	015519-14-9	47
5	Butyric acid, 2-pentadecyl ester			298	C19H38O2	107853-73-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042121\
Data File : BG048830.D
Acq On : 21 Apr 2021 22:07
Operator : CG/JU
Sample : M1998-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
SB-4A

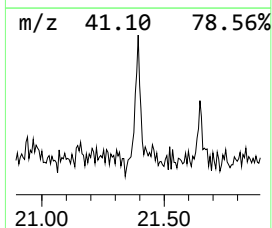
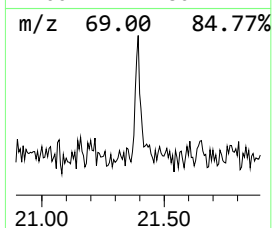
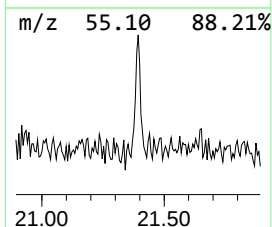
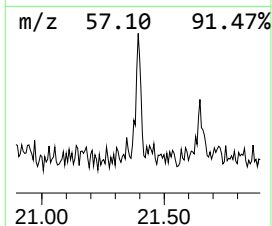
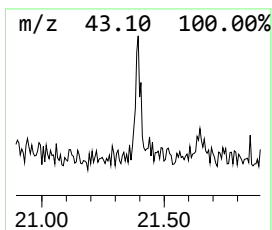
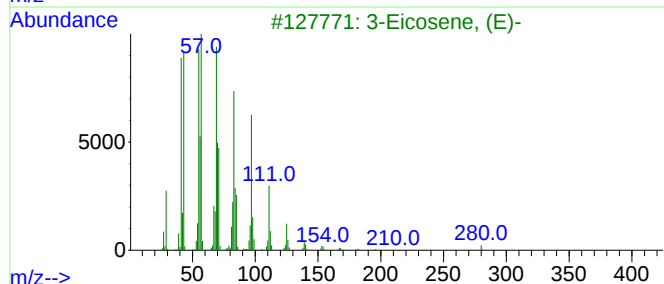
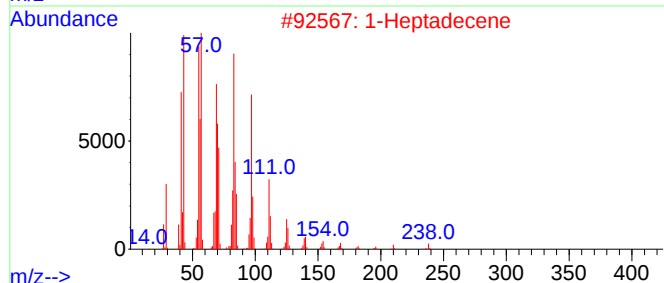
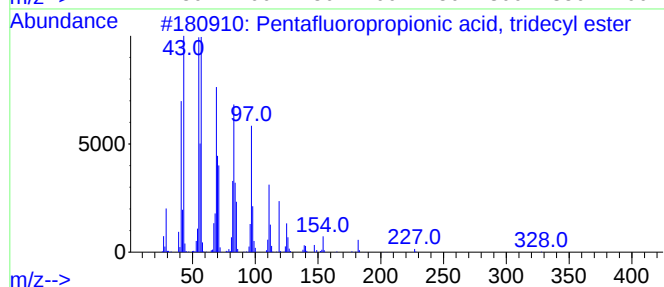
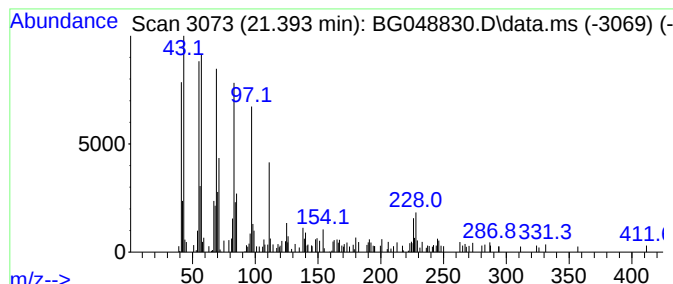
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.393	5.06 ng	101511	Chrysene-d12	21.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	87
2			1-Heptadecene	238	C17H34	006765-39-5	87
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	83
4			11-Methyldodecanol	200	C13H28O	085763-57-1	80
5			5-Eicosene, (E)-	280	C20H40	074685-30-6	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042121\
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Operator : CG/JU
Sample : M1998-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-4A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.130	15.7	ng	130533	1	8.056	165903	20.0
unknown8.115	8.115	2.0	ng	16844	1	8.056	165903	20.0
2-Piperidinone	10.588	2.4	ng	28541	2	10.888	238947	20.0
Indole	12.380	10.4	ng	123979	2	10.888	238947	20.0
unknown17.551	17.551	2.5	ng	49438	4	17.480	388535	20.0
Phytol	19.366	3.3	ng	64361	4	17.480	388535	20.0
Pentafluoroprop...	21.393	5.1	ng	101511	5	21.775	401624	20.0