

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
 Data File : BG048841.D
 Acq On : 22 Apr 2021 10:59
 Operator : CG/JU
 Sample : M2111-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S-4

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: BG048841.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.612	380	387	396	rVB	244135	393177	41.50%	6.609%
2	7.222	653	661	676	rBV	249784	443734	46.84%	7.459%
3	8.062	797	804	810	rBV2	76157	126340	13.34%	2.124%
4	9.237	996	1004	1013	rBV	165334	293843	31.02%	4.939%
5	10.888	1278	1285	1292	rBV2	91453	163627	17.27%	2.750%
6	13.338	1695	1702	1711	rVB	400022	591437	62.43%	9.941%
7	13.603	1741	1747	1755	rBV2	47134	68151	7.19%	1.146%
8	14.167	1837	1843	1848	rBV	20792	30462	3.22%	0.512%
9	14.725	1929	1938	1946	rBV2	141580	227263	23.99%	3.820%
10	15.823	2119	2125	2136	rBV3	29956	45264	4.78%	0.761%
11	16.217	2186	2192	2202	rBV	329409	512589	54.11%	8.616%
12	17.480	2401	2407	2412	rBV	204348	292968	30.93%	4.924%
13	17.516	2412	2413	2420	rVB3	6136	10166	1.07%	0.171%
14	17.768	2451	2456	2463	rBV3	8525	15908	1.68%	0.267%
15	18.362	2553	2557	2561	rBV4	15934	26308	2.78%	0.442%
16	19.425	2734	2738	2739	rBV4	9022	11727	1.24%	0.197%
17	19.484	2739	2748	2751	rBV2	48283	102461	10.82%	1.722%
18	19.731	2777	2790	2795	rBV9	15673	62393	6.59%	1.049%
19	19.895	2815	2818	2825	rVB2	23415	33346	3.52%	0.561%
20	20.089	2846	2851	2857	rVB	725072	947309	100.00%	15.923%
21	20.212	2864	2872	2873	rBV6	28177	47248	4.99%	0.794%
22	20.383	2900	2901	2906	rVB5	12677	11542	1.22%	0.194%
23	20.882	2982	2986	2990	rVB7	11122	16273	1.72%	0.274%
24	21.170	3026	3035	3046	rBV3	72638	239286	25.26%	4.022%
25	21.341	3061	3064	3067	rBV4	7907	12463	1.32%	0.209%
26	21.393	3069	3073	3078	rVV4	55999	75784	8.00%	1.274%
27	21.493	3086	3090	3092	rBV5	7340	10238	1.08%	0.172%
28	21.775	3132	3138	3144	rBV	209028	355033	37.48%	5.968%
29	21.822	3144	3146	3152	rVB6	11530	18081	1.91%	0.304%
30	21.963	3165	3170	3172	rBV5	8629	13061	1.38%	0.220%
31	22.586	3272	3276	3280	rBV5	10196	16738	1.77%	0.281%
32	22.833	3308	3318	3330	rBV5	51723	189938	20.05%	3.193%
33	22.974	3338	3342	3345	rBV6	13365	17446	1.84%	0.293%
34	23.503	3428	3432	3441	rVB9	12164	28778	3.04%	0.484%
35	24.137	3534	3540	3551	rVB9	21356	55287	5.84%	0.929%
36	24.848	3654	3661	3662	rBV6	24261	39027	4.12%	0.656%

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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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37	25.118	3696	3707	3718	rVB2	118368	351900	37.15%	5.915%
38	26.135	3872	3880	3881	rBV6	11568	24241	2.56%	0.407%
39	26.288	3901	3906	3907	rBV5	10833	14866	1.57%	0.250%
40	27.287	4071	4076	4077	rBV4	8385	13593	1.43%	0.228%

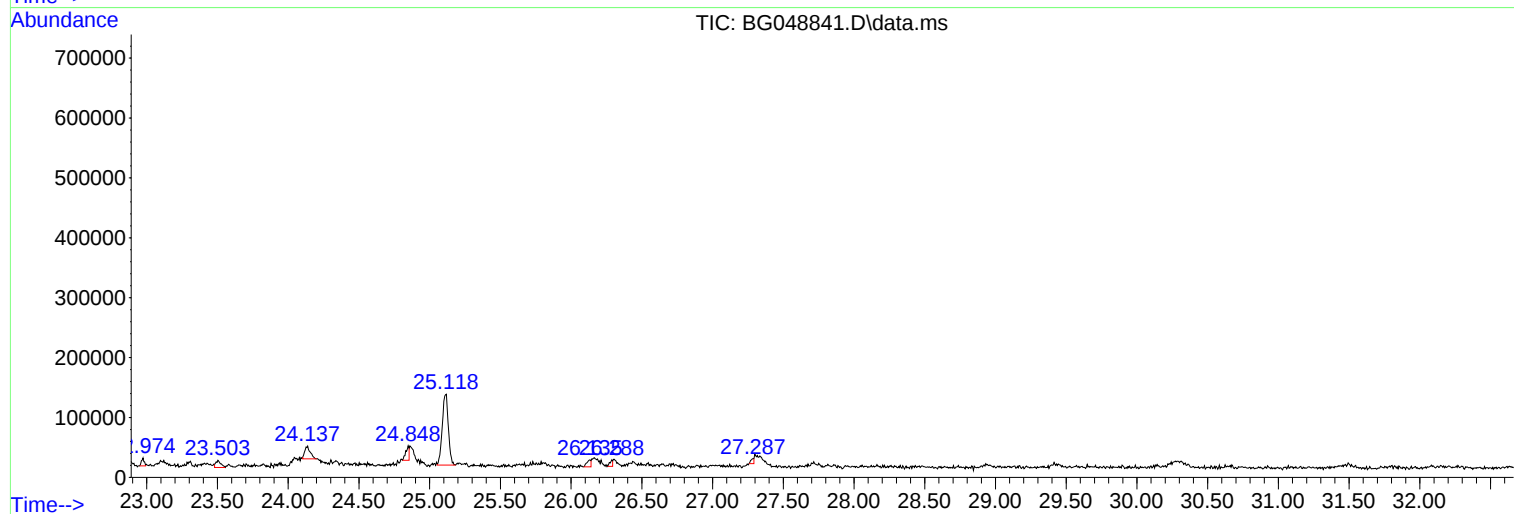
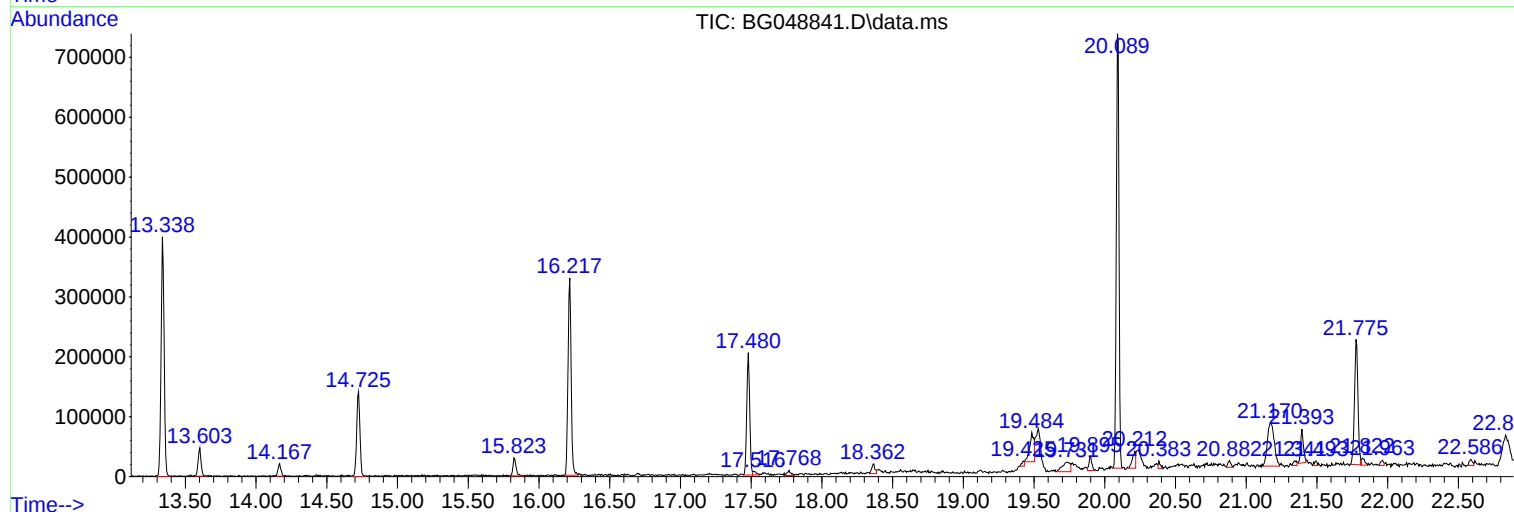
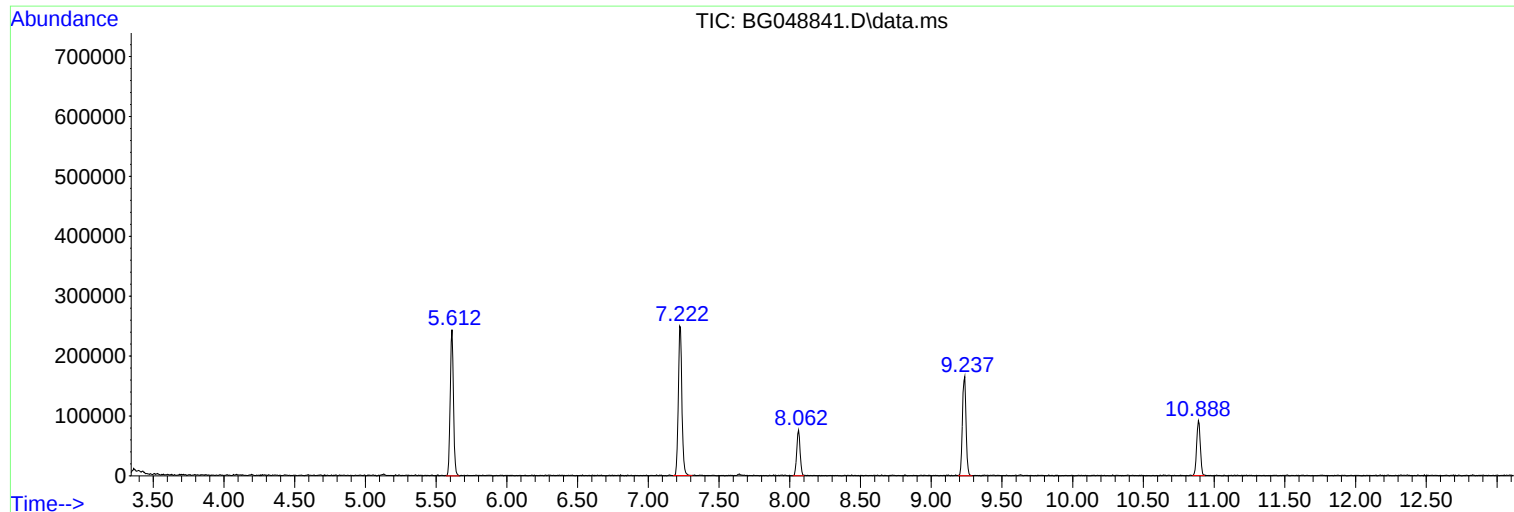
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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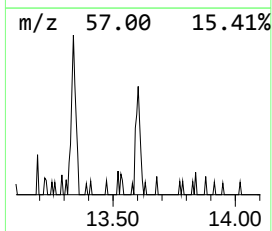
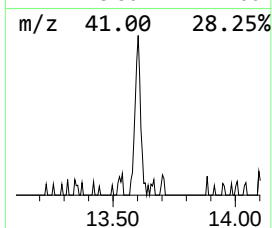
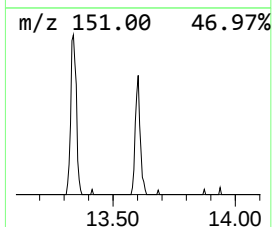
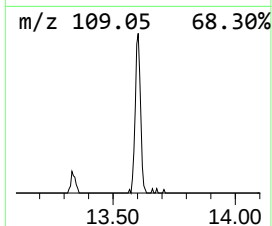
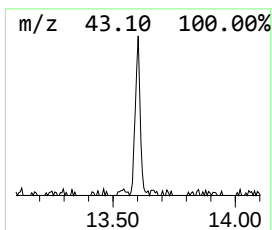
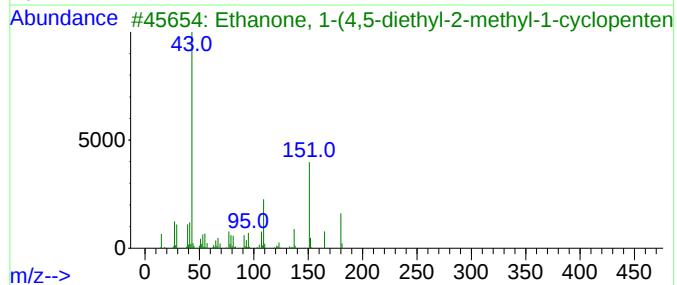
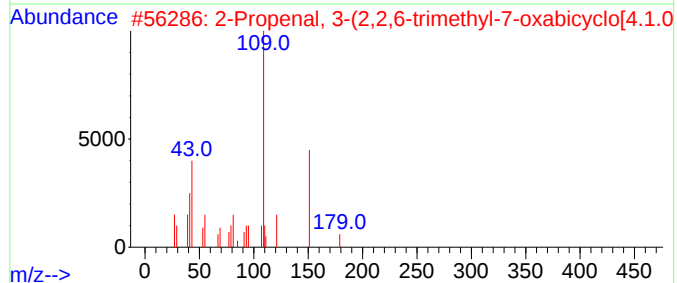
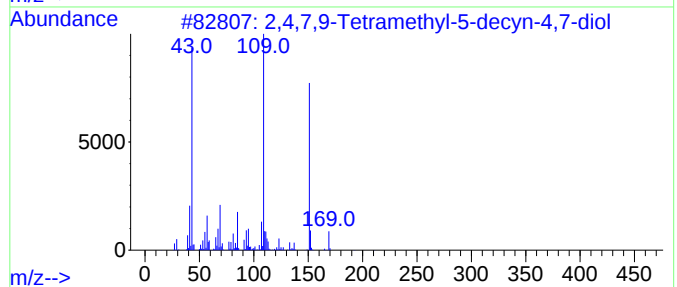
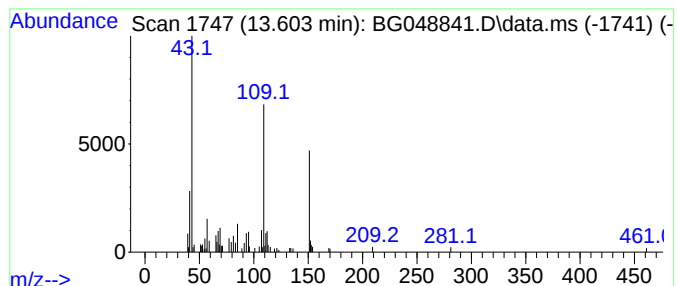
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.602	6.00 ng	68151	Acenaphthene-d10	14.725

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	80	
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	59	
3	Ethanone, 1-(4,5-diethyl-2-methy...	180	C12H20O	062338-24-3	50	
4	Metacetamol	151	C8H9NO2	000621-42-1	40	
5	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	40	



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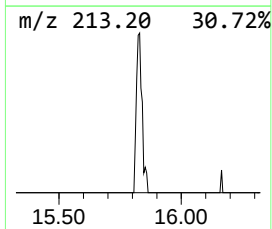
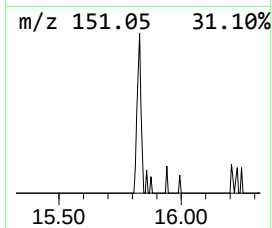
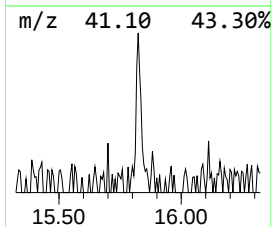
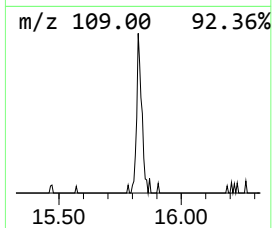
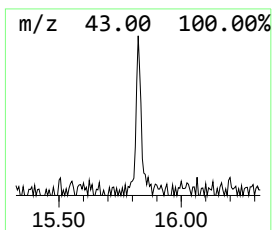
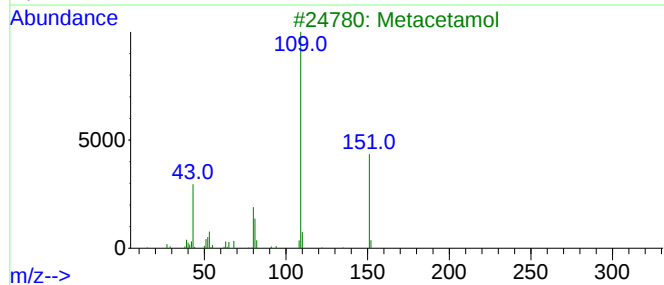
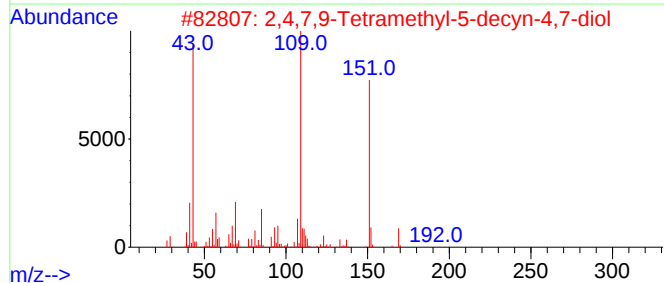
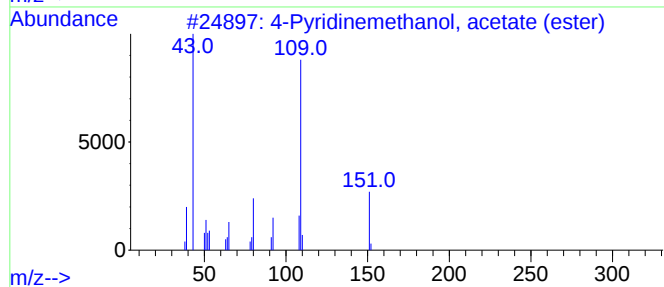
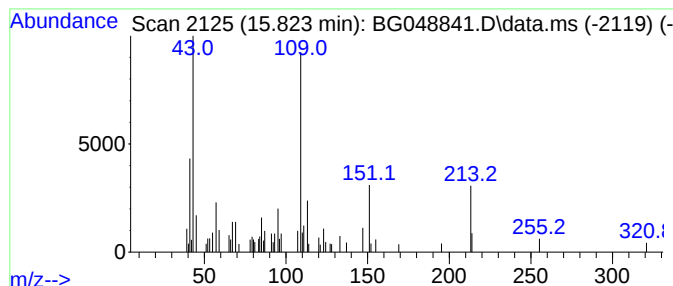
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown15.82 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.823	3.98 ng	45264	Acenaphthene-d10	14.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	43
2			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	43
3			Metacetamol	151	C8H9NO2	000621-42-1	38
4			Acetamide, N-(2-hydroxyphenyl)-	151	C8H9NO2	000614-80-2	38
5			m-Isopropoxyaniline	151	C9H13NO	041406-00-2	38



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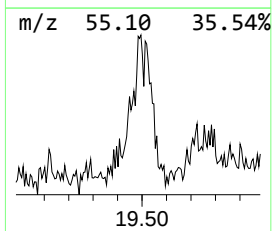
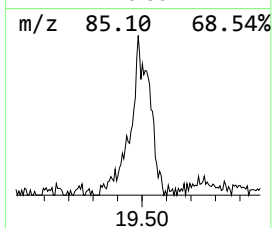
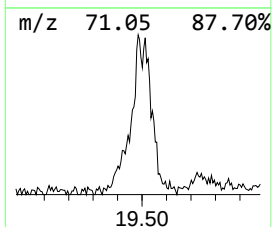
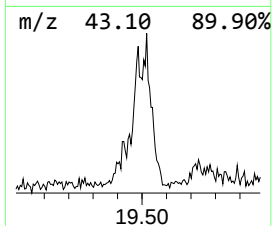
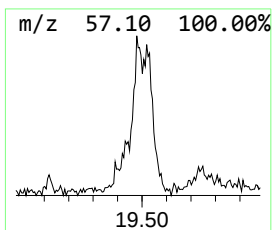
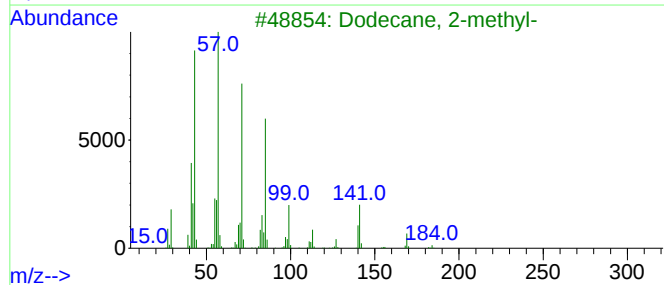
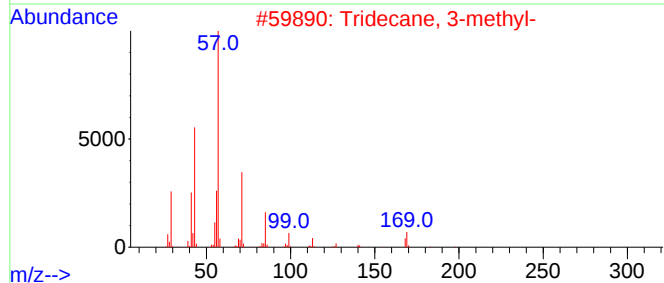
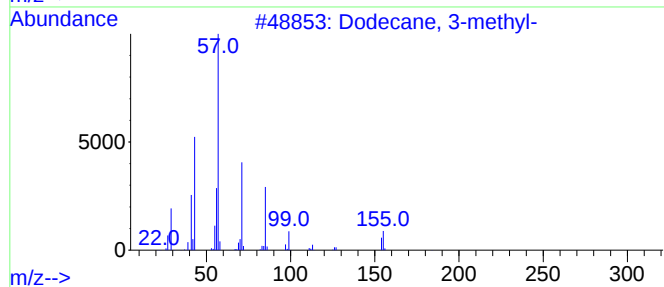
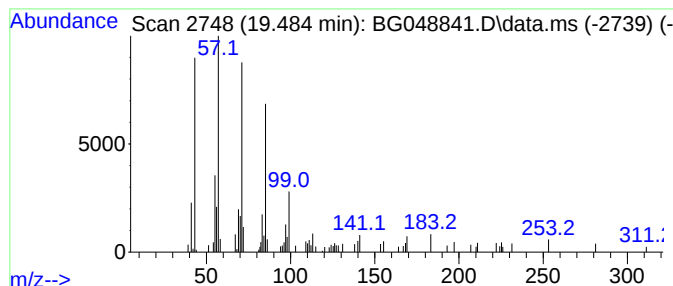
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.484	6.99 ng	102461	Phenanthrene-d10	17.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 3-methyl-	184	C13H28	017312-57-1	86
2			Tridecane, 3-methyl-	198	C14H30	006418-41-3	86
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
4			Heptadecane, 2,3-dimethyl-	268	C19H40	061868-03-9	72
5			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	72



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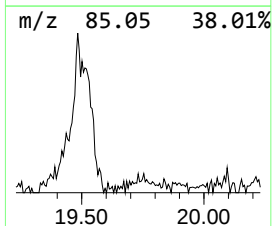
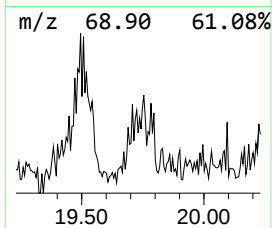
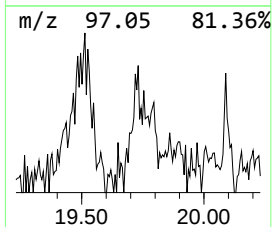
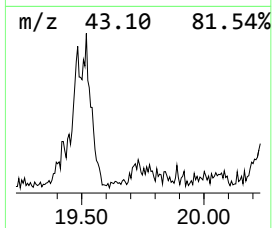
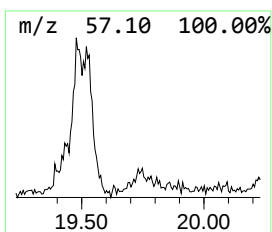
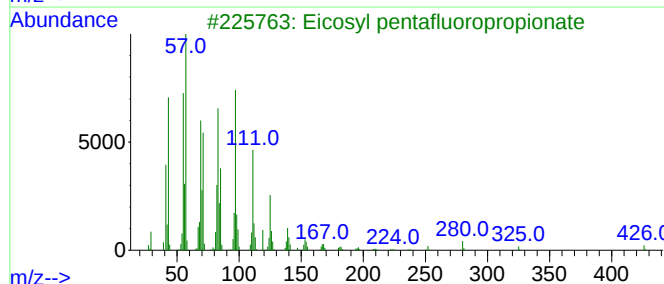
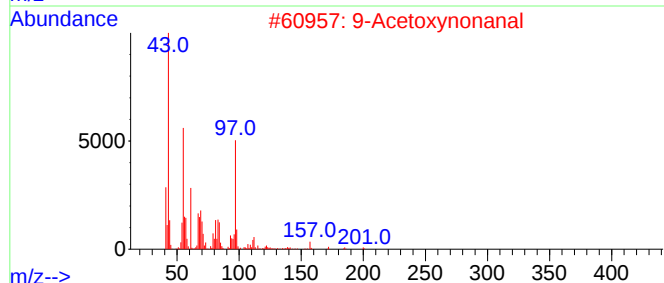
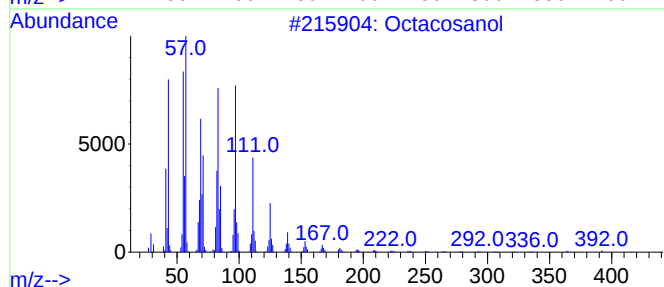
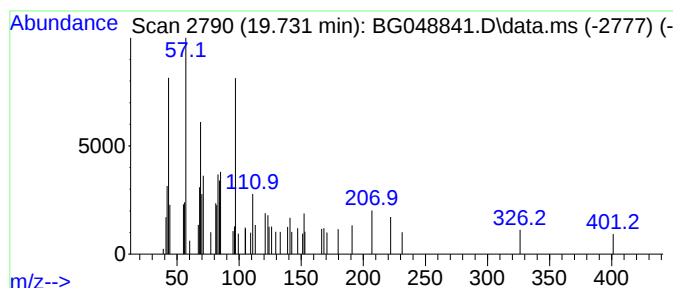
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown19.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.731	3.51 ng	62393	Chrysene-d12	21.775	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	38
2	9-Acetoxynonanal	200	C11H20O3	029541-97-7	35
3	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	27
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	27
5	1-Heptacosanol	396	C27H56O	002004-39-9	22



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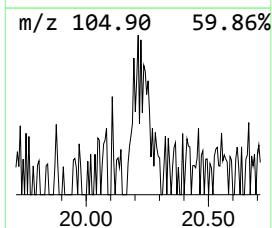
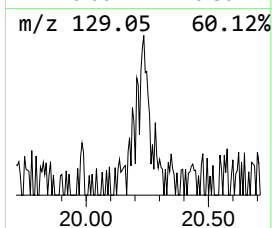
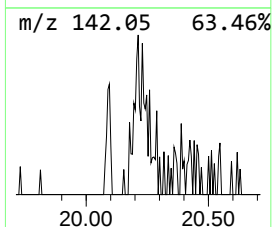
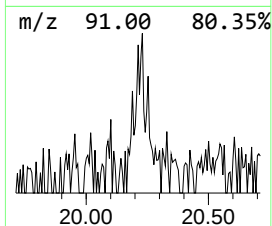
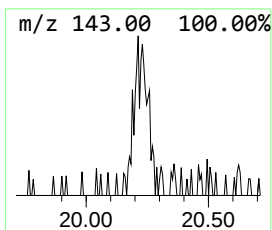
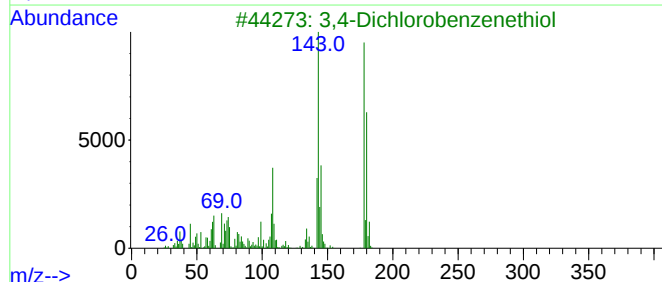
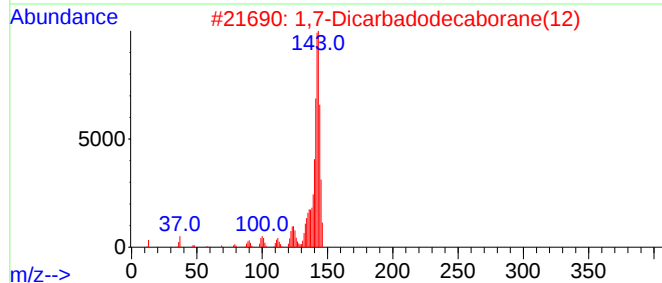
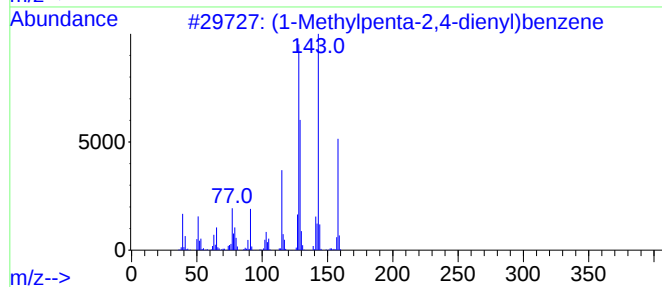
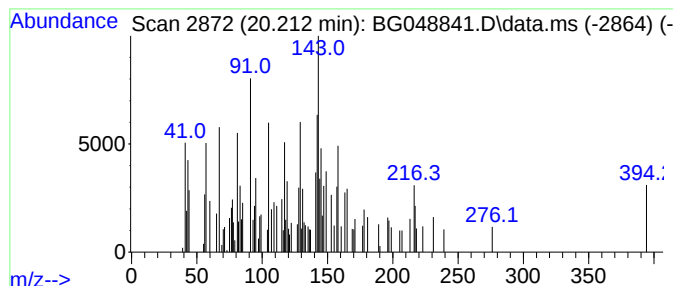
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown20.21 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.212	2.66 ng	47248	Chrysene-d12	21.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1-Methylpenta-2,4-dienyl)benzene	158	C12H14	1000210-01-1	43		
2	1,7-Dicarbadodecaborane(12)	146	C2H12B10	016986-24-6	41		
3	3,4-Dichlorobenzenethiol	178	C6H4Cl2S	005858-17-3	30		
4	1H-Pyrazole, 5-chloro-1-methyl-3...	158	C7H11ClN2	1000319-90-4	30		
5	3-Heptyne, 7-chloro-2,2-dimethyl-	158	C9H15Cl	055402-10-3	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048841.D
Acq On : 22 Apr 2021 10:59
Operator : CG/JU
Sample : M2111-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S-4

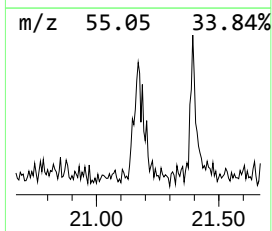
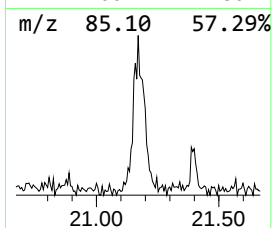
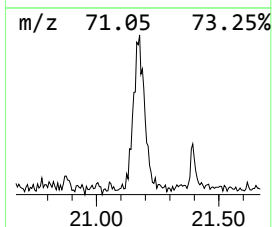
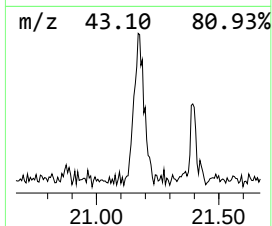
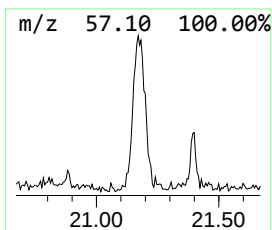
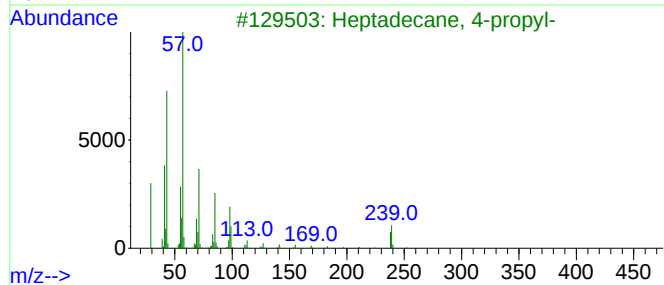
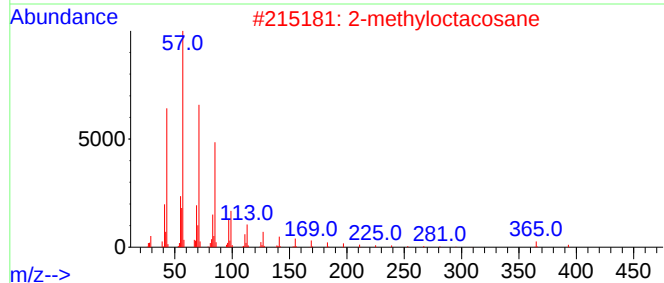
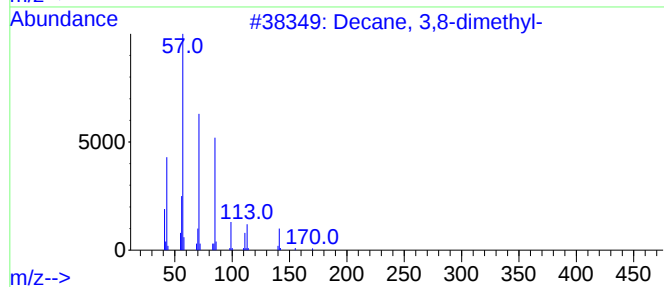
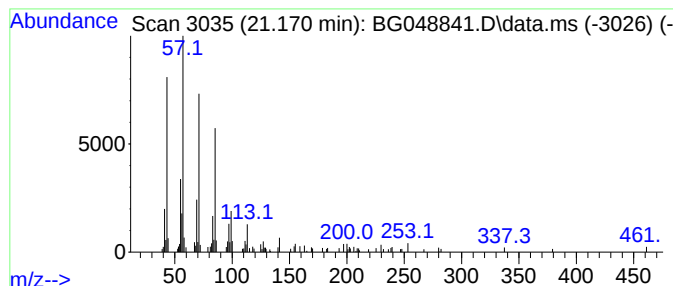
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Decane, 3,8-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.170	13.48 ng	239286	Chrysene-d12	21.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
2			2-methyloctacosane	408	C29H60	1000376-72-8	87
3			Heptadecane, 4-propyl-	282	C20H42	055044-10-5	87
4			Heneicosane	296	C21H44	000629-94-7	86
5			Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048841.D
Acq On : 22 Apr 2021 10:59
Operator : CG/JU
Sample : M2111-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

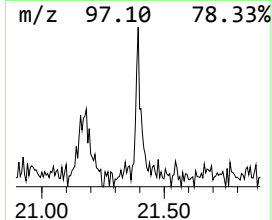
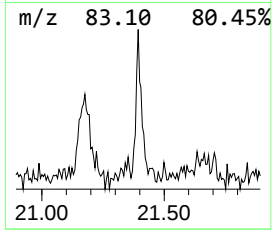
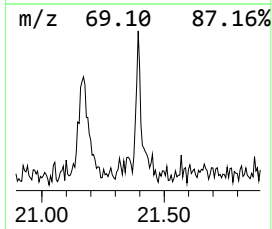
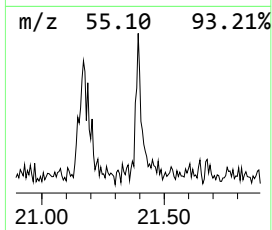
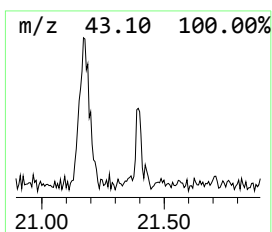
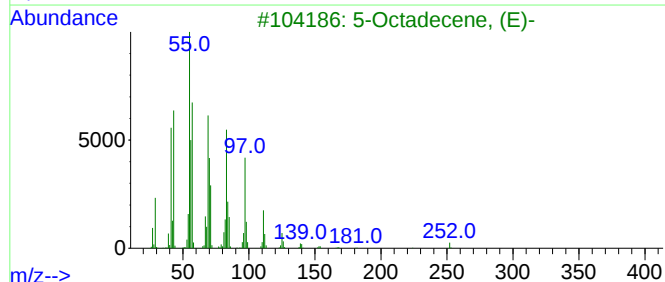
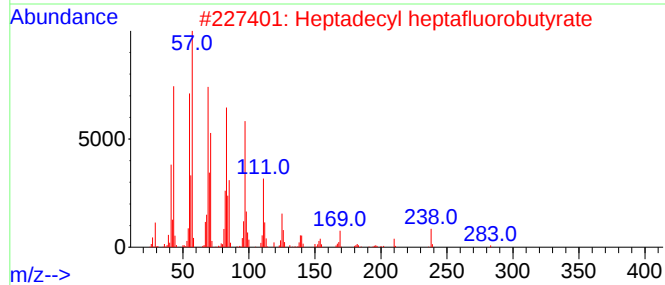
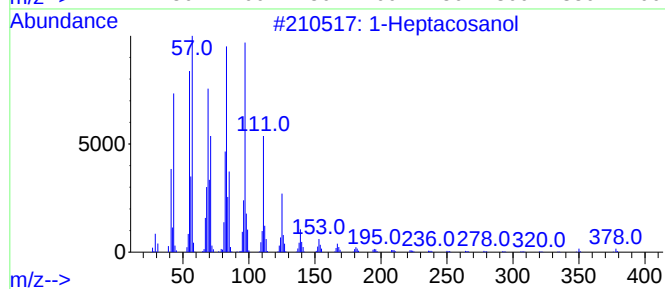
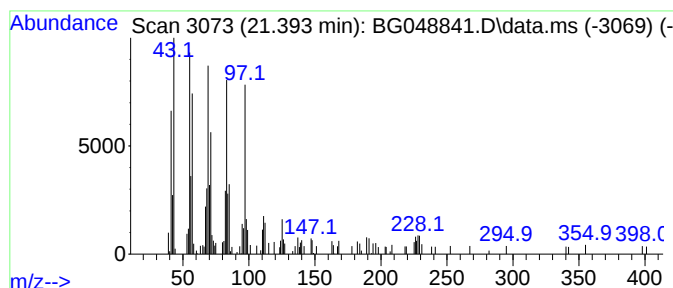
Instrument :
BNA_G
ClientSampled :
S-4

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 7 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.393	4.27 ng	75784	Chrysene-d12	21.775	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	90
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
5	1-Octadecene	252	C18H36	000112-88-9	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048841.D
Acq On : 22 Apr 2021 10:59
Operator : CG/JU
Sample : M2111-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
S-4

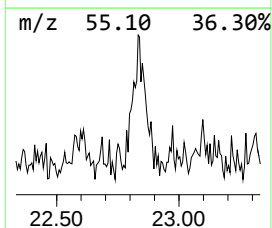
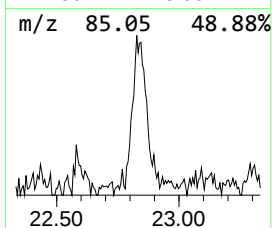
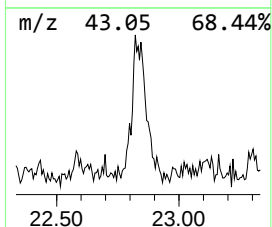
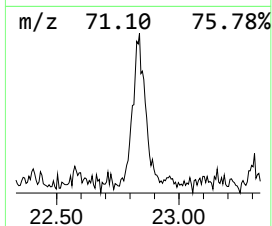
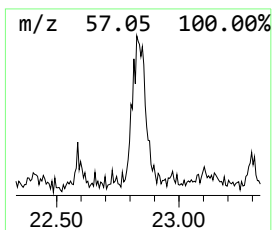
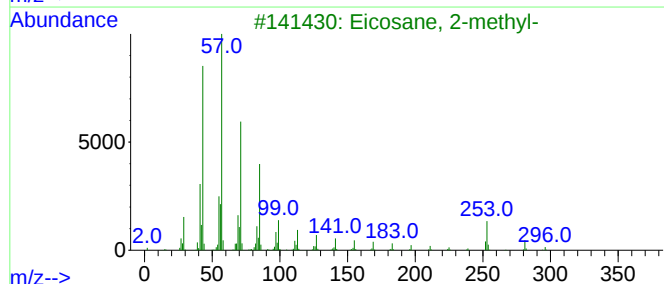
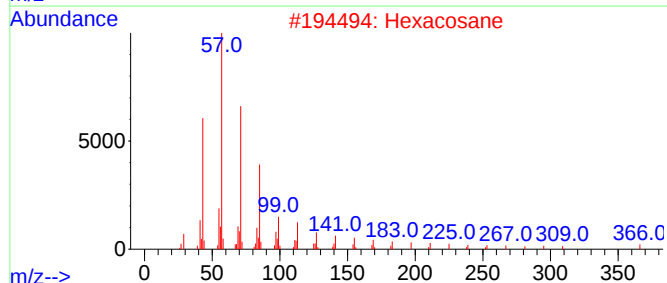
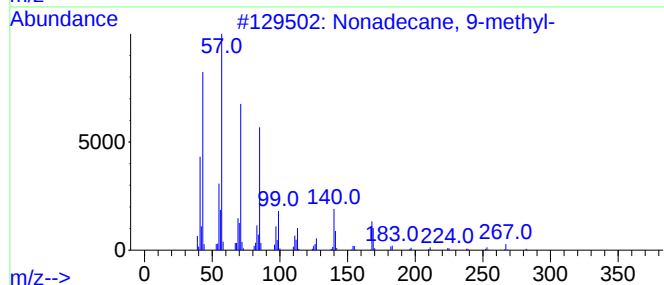
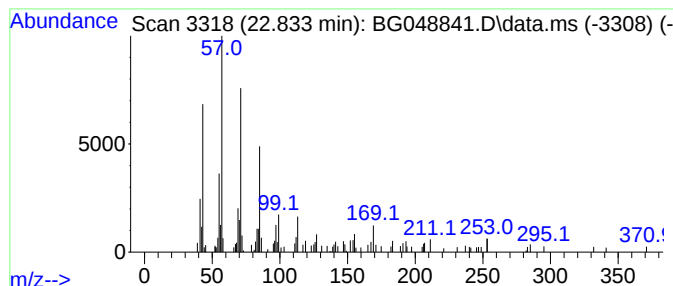
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane, 9-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.833	10.70 ng	189938	Chrysene-d12	21.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2			Hexacosane	366	C26H54	000630-01-3	90
3			Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
4			Eicosane	282	C20H42	000112-95-8	86
5			Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048841.D
Acq On : 22 Apr 2021 10:59
Operator : CG/JU
Sample : M2111-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
S-4

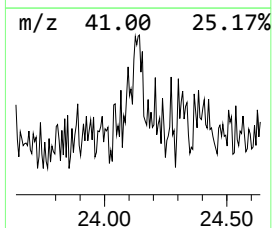
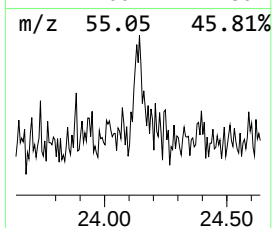
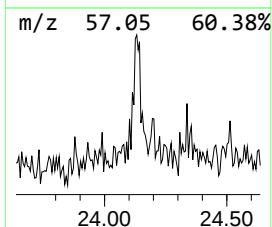
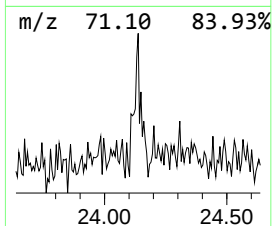
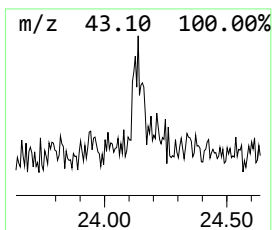
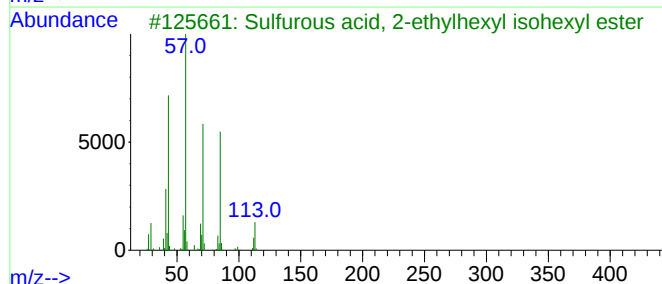
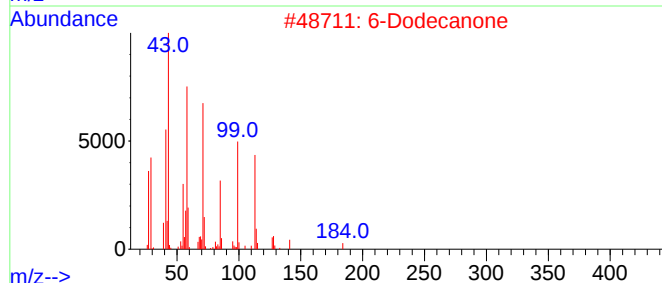
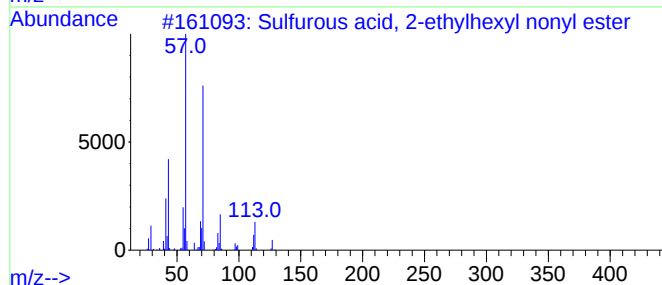
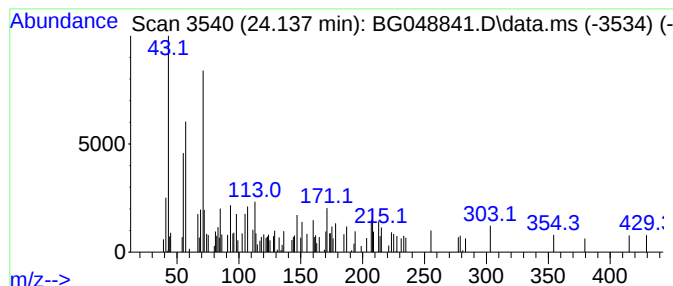
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown24.13 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.137	3.14 ng	55287	Perylene-d12	25.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	43
2			6-Dodecanone	184	C12H24O	006064-27-3	43
3			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	37
4			1-Methylcycloheptanol	128	C8H16O	003761-94-2	37
5			Acetic acid, 4-methyl-3-oxopent-...	156	C8H12O3	1000191-76-4	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048841.D
Acq On : 22 Apr 2021 10:59
Operator : CG/JU
Sample : M2111-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
S-4

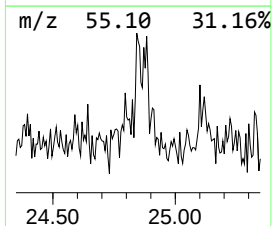
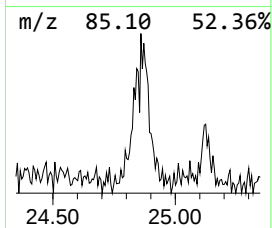
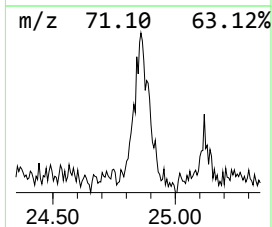
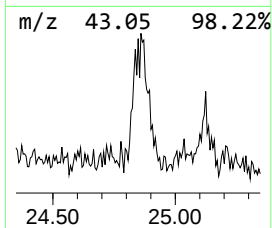
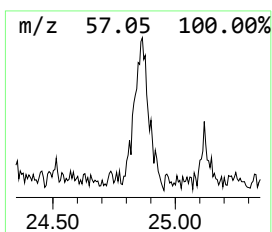
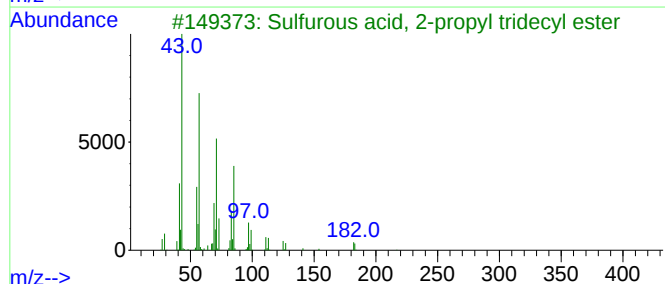
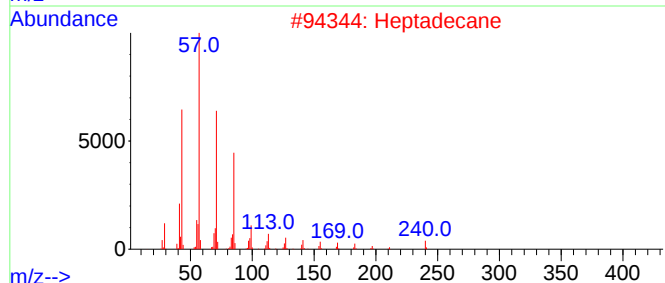
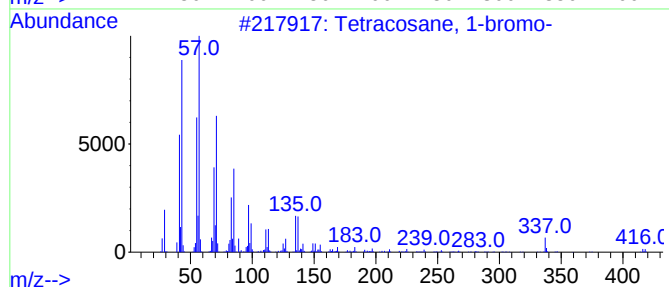
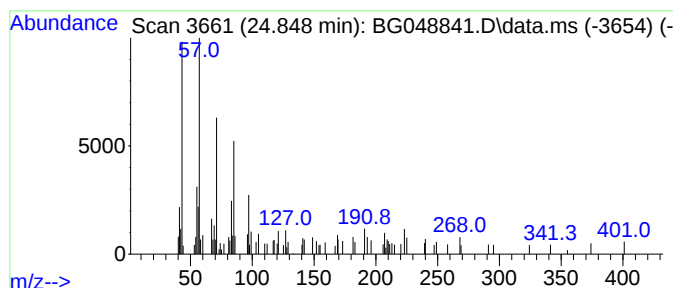
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane, 1-bromo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.848	2.22 ng	39027	Perylene-d12	25.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane, 1-bromo-	416	C24H49Br	006946-24-3	59
2			Heptadecane	240	C17H36	000629-78-7	53
3			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	52
4			2-methylhexacosane	380	C27H56	1000376-72-7	52
5			2-methyltetracosane	352	C25H52	1000376-72-6	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042221\
Data File : BG048841.D
Acq On : 22 Apr 2021 10:59
Operator : CG/JU
Sample : M2111-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown15.82	15.823	4.0	ng	45264	3	14.725	227263	20.0
Dodecane, 3-met...	19.484	7.0	ng	102461	4	17.480	292968	20.0
unknown19.73	19.731	3.5	ng	62393	5	21.775	355033	20.0
unknown20.21	20.212	2.7	ng	47248	5	21.775	355033	20.0
Decane, 3,8-dim...	21.170	13.5	ng	239286	5	21.775	355033	20.0
1-Heptacosanol	21.393	4.3	ng	75784	5	21.775	355033	20.0
Nonadecane, 9-m...	22.833	10.7	ng	189938	5	21.775	355033	20.0
unknown24.13	24.137	3.1	ng	55287	6	25.107	351900	20.0
Tetracosane, 1-...	24.848	2.2	ng	39027	6	25.107	351900	20.0