

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122223\
 Data File : BG060141.D
 Acq On : 22 Dec 2023 16:51
 Operator : MA/JU
 Sample : 05900-22
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-64a

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-BG122123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060141.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.120	3	5	10	rVB	245217	271390	2.04%	0.367%
2	5.511	405	412	429	rBV	3101070	5249998	39.39%	7.090%
3	7.104	674	683	701	rBV	3774968	6559475	49.22%	8.858%
4	7.938	817	825	835	rBV	794232	1370776	10.29%	1.851%
5	9.101	1015	1023	1034	rBV	2019859	3638157	27.30%	4.913%
6	10.746	1294	1303	1316	rBV	1204857	2271660	17.05%	3.068%
7	13.202	1712	1721	1731	rBV	6273136	9895933	74.25%	13.364%
8	14.577	1948	1955	1963	rBV	2541723	3915590	29.38%	5.288%
9	16.064	2201	2208	2220	rBV	5365895	8191512	61.47%	11.062%
10	17.327	2415	2423	2433	rBV	3273471	5166225	38.76%	6.977%
11	18.214	2570	2574	2582	rBV	519868	743286	5.58%	1.004%
12	19.942	2862	2868	2882	rBV	9649128	13327097	100.00%	17.998%
13	20.271	2921	2924	2927	rVB2	116047	133760	1.00%	0.181%
14	20.453	2950	2955	2962	rBV	117046	185453	1.39%	0.250%
15	20.823	3014	3018	3022	rVB5	117611	165460	1.24%	0.223%
16	21.234	3084	3088	3097	rBV	594556	906473	6.80%	1.224%
17	21.410	3115	3118	3125	rVB7	72496	133732	1.00%	0.181%
18	21.516	3133	3136	3141	rBV2	135048	205138	1.54%	0.277%
19	21.587	3141	3148	3156	rVB2	3210099	5227333	39.22%	7.059%
20	22.068	3225	3230	3236	rVB	125298	199021	1.49%	0.269%
21	22.397	3280	3286	3295	rVB4	184081	471231	3.54%	0.636%
22	23.860	3530	3535	3540	rBV2	108842	227800	1.71%	0.308%
23	23.919	3540	3545	3556	rVB2	226641	525453	3.94%	0.710%
24	24.236	3594	3599	3607	rVB8	59865	144605	1.09%	0.195%
25	24.765	3679	3689	3703	rVB	1454661	4129443	30.99%	5.577%
26	26.034	3899	3905	3916	rVB9	113012	329727	2.47%	0.445%
27	28.690	4349	4357	4368	rVB8	128195	463089	3.47%	0.625%

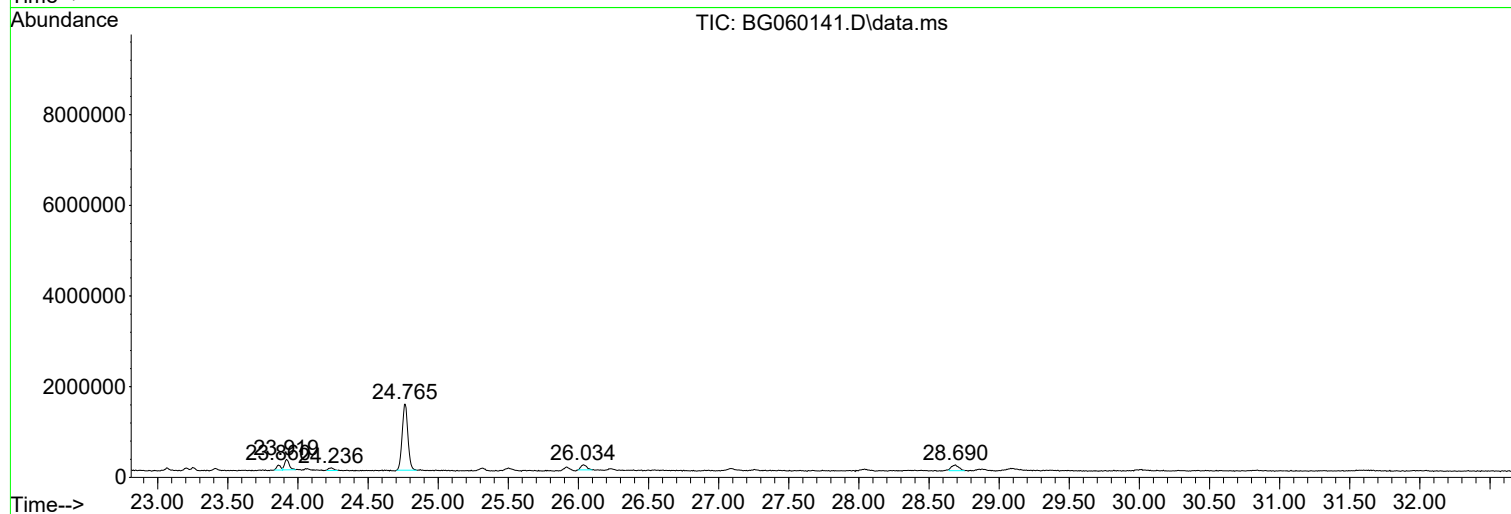
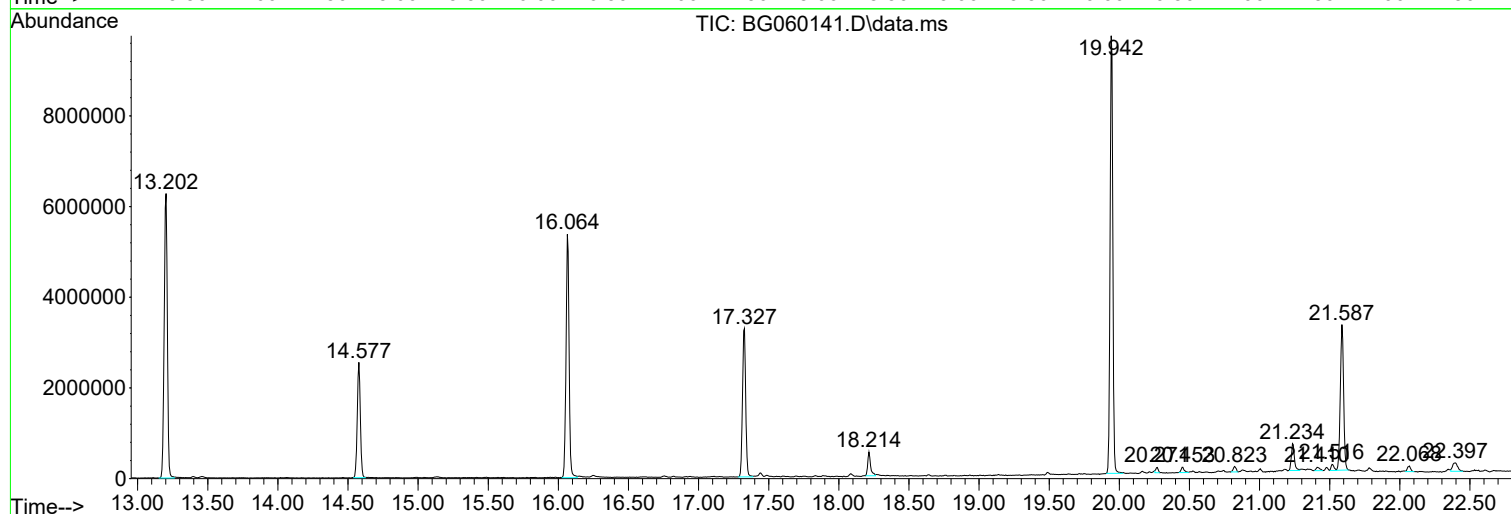
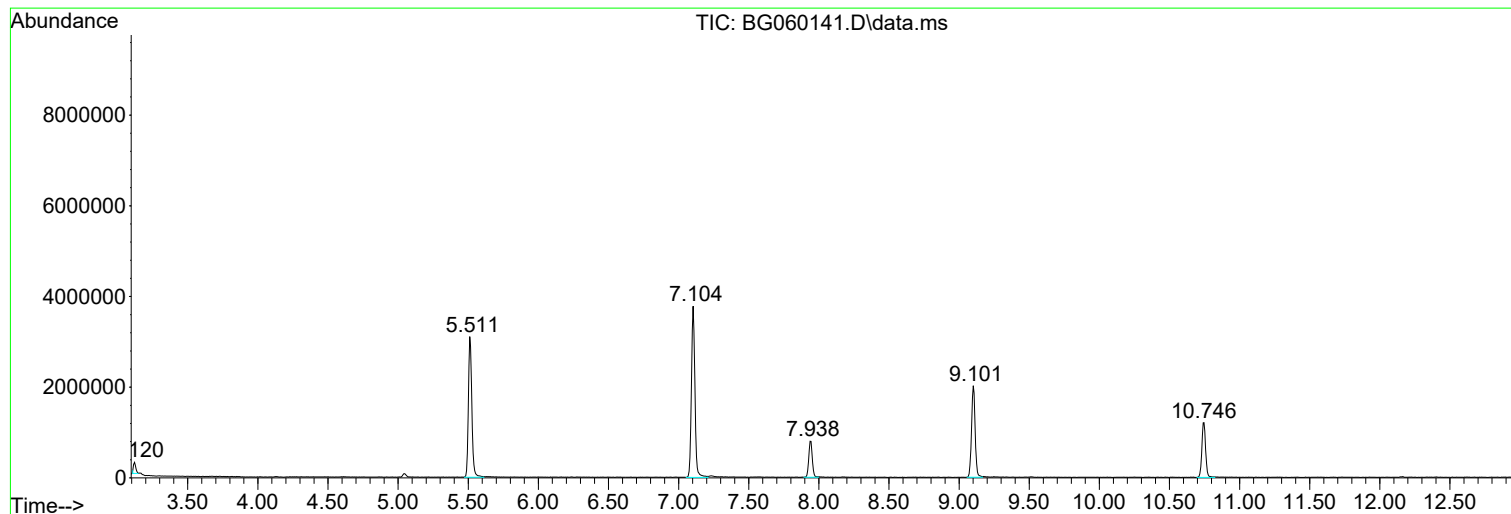
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ClientSampleId :
GHL-SS-64a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.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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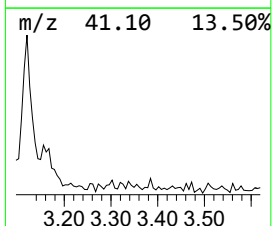
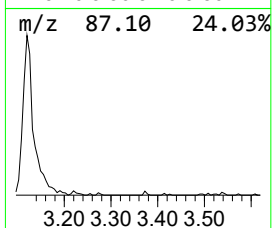
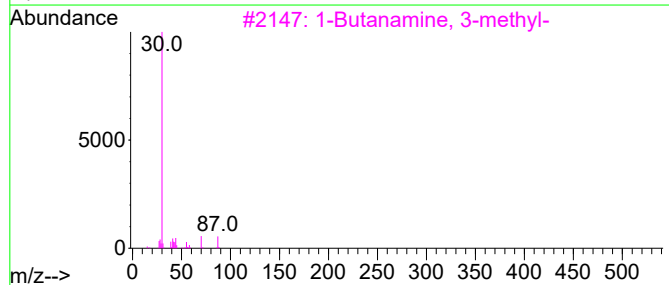
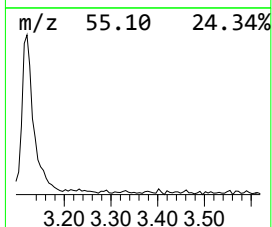
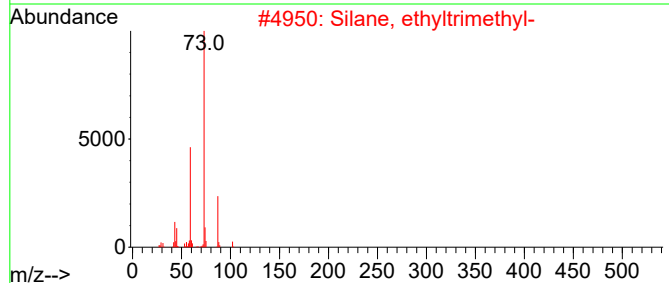
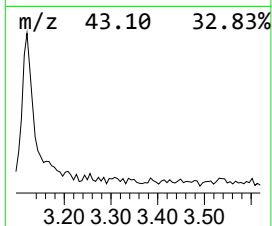
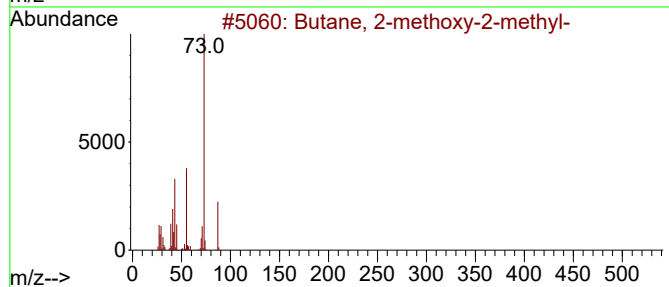
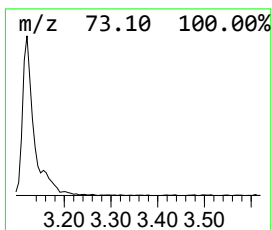
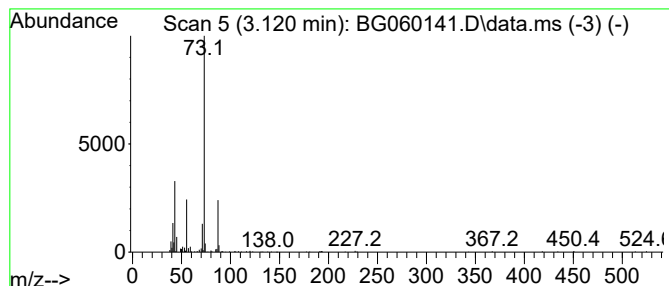
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.120	3.96 ng	271390	1,4-Dichlorobenzene-d4	7.944

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	28
3		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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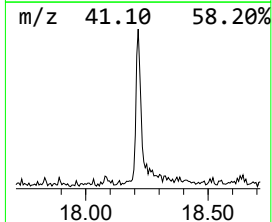
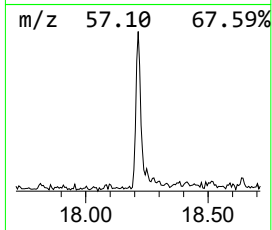
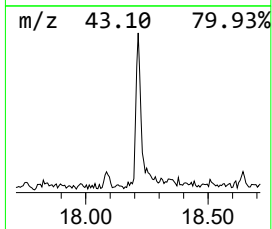
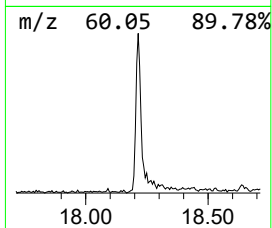
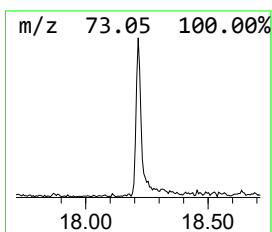
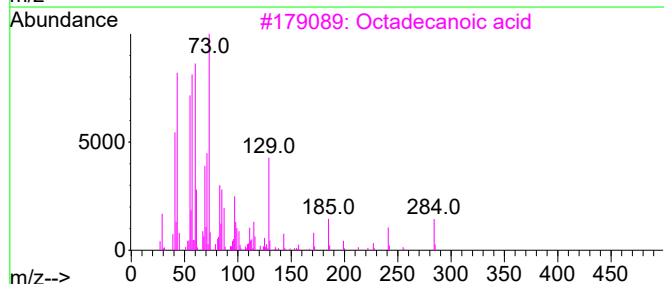
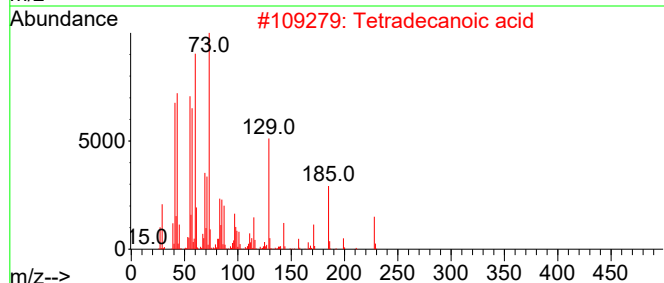
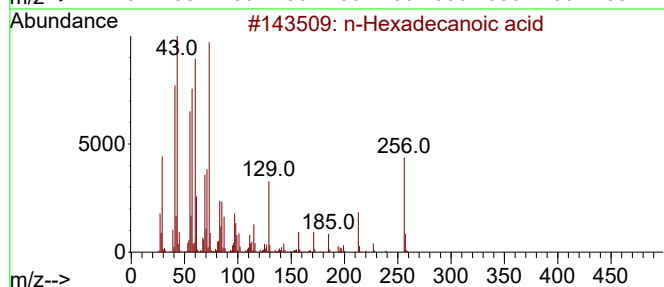
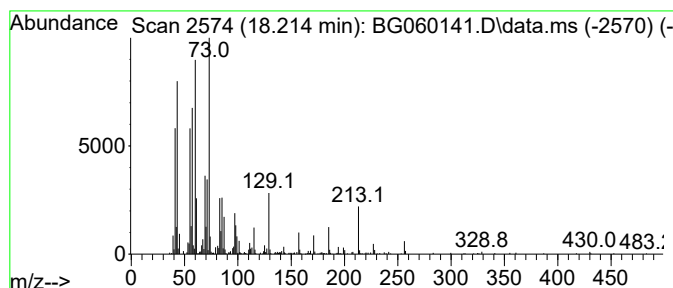
Instrument :
BNA_G
ClientSampleId :
GHL-SS-64a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.214	2.88 ng	743286	Phenanthrene-d10	17.321	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Octanoic acid	144	C8H16O2	000124-07-2	60



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ClientSampleId :
GHL-SS-64a

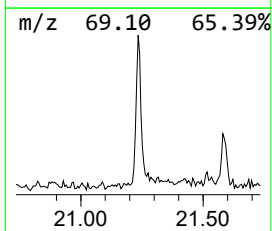
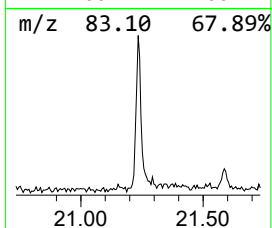
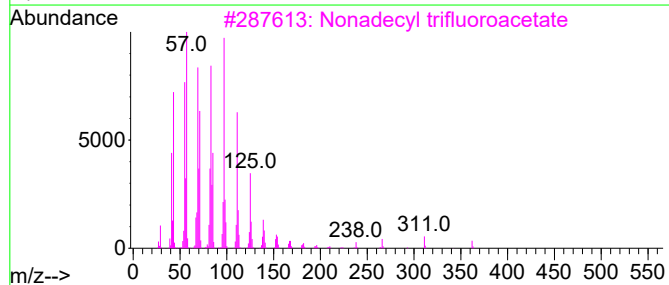
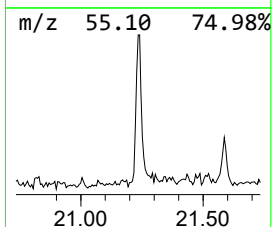
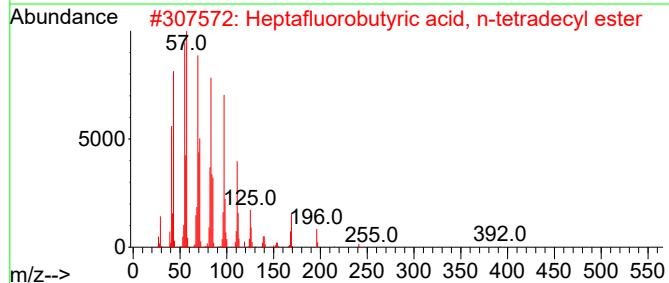
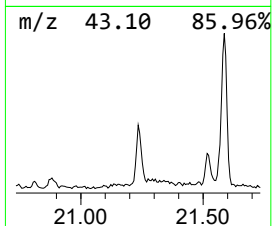
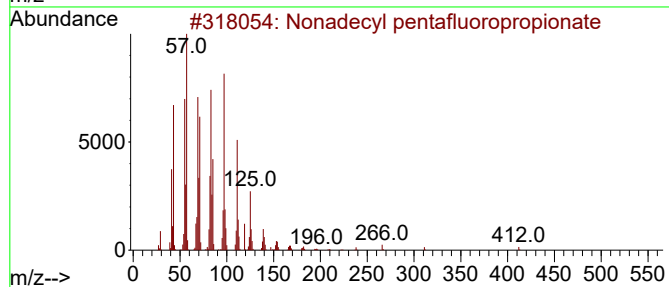
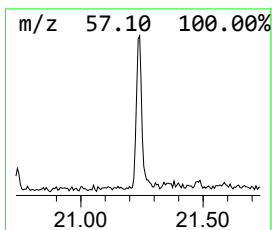
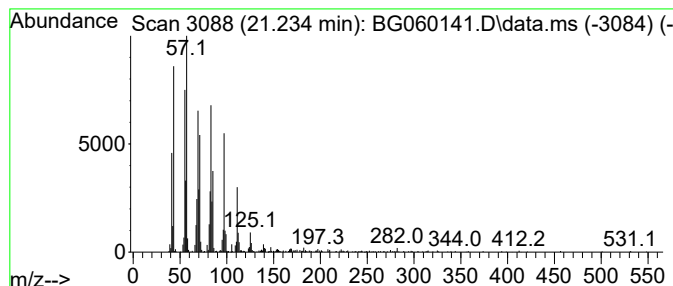
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Nonadecyl pentafluoropropio... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.234	3.47 ng	906473	Chrysene-d12	21.587

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	87
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	81
5			1-Heneicosanol	312	C21H44O	015594-90-8	81



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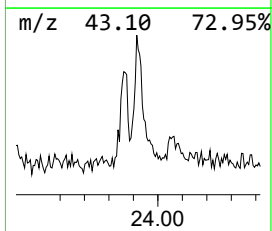
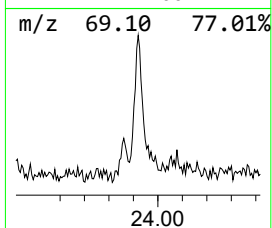
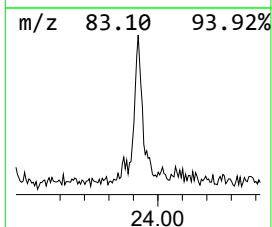
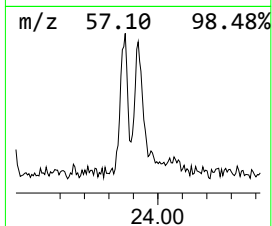
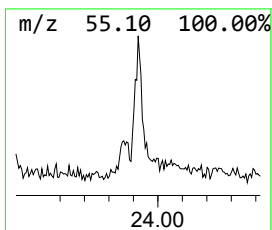
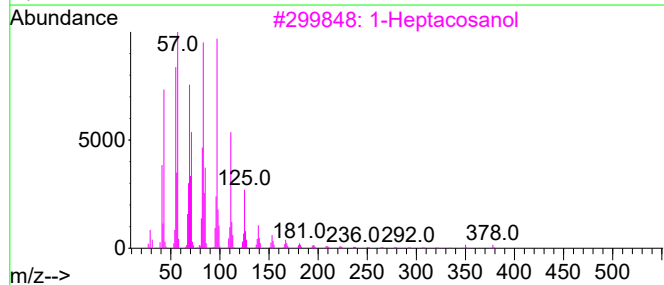
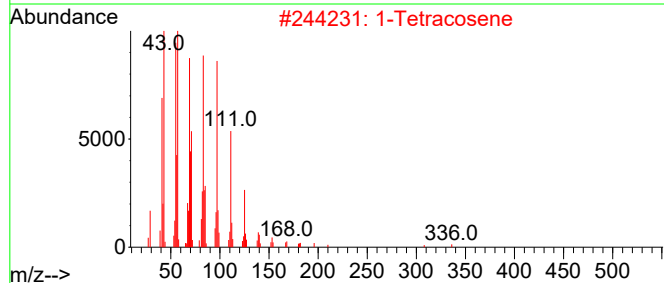
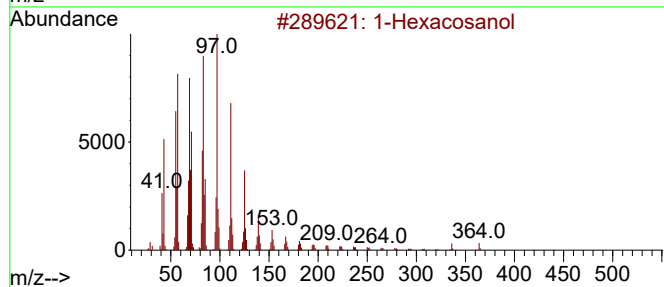
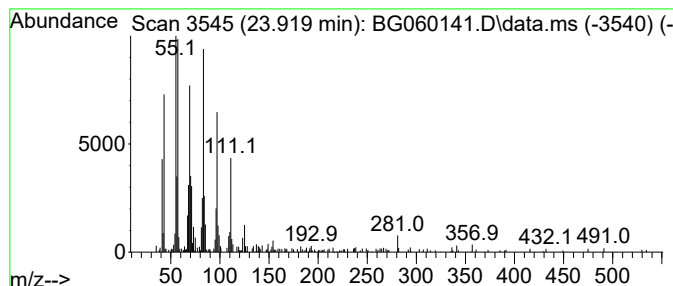
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.919	2.54 ng	525453	Perylene-d12	24.765

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexacosanol	382	C26H54O	000506-52-5	90
2		1-Tetracosene	336	C24H48	010192-32-2	87
3		1-Heptacosanol	396	C27H56O	002004-39-9	80
4		Henicos-1-ene	294	C21H42	001599-68-4	70
5		Cyclotetracosane	336	C24H48	000297-03-0	58



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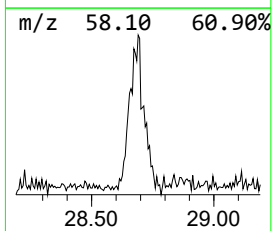
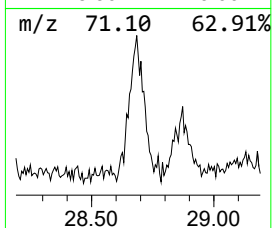
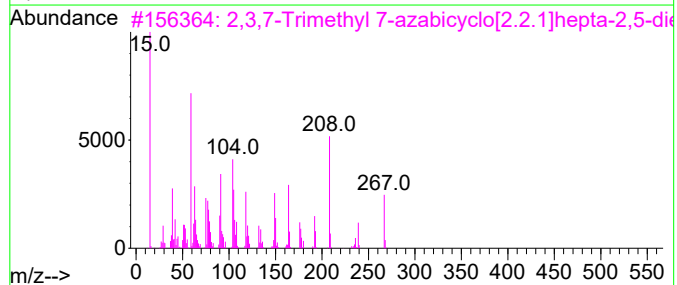
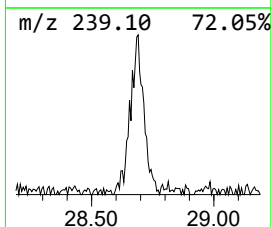
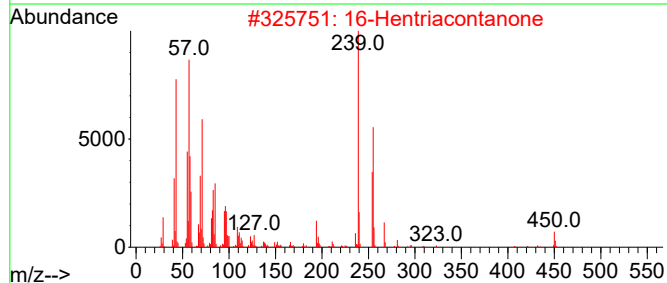
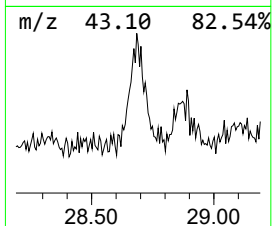
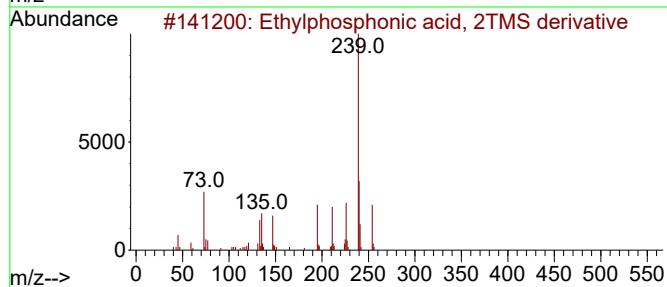
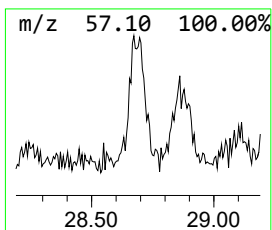
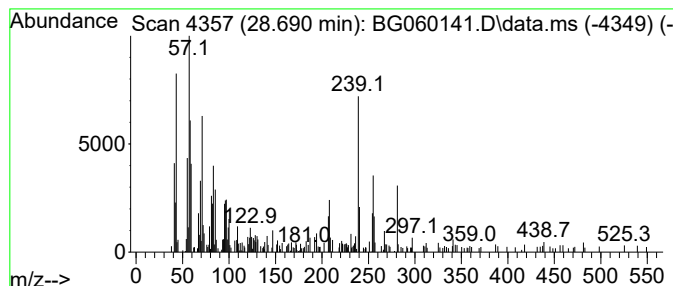
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown28.690 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.690	2.24 ng	463089	Perylene-d12	24.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylphosphonic acid, 2TMS deriv...	254	C8H23O3PSi2	001641-57-2	30
2			16-Hentriacontanone	450	C31H62O	000502-73-8	27
3			2,3,7-Trimethyl 7-azabicyclo[2.2...	267	C12H13N06	1000411-57-6	27
4			Ethyl 3,6-dihydroxy-6-methyl-4-(...	330	C18H22N2O4	1000389-06-2	25
5			16-Hexadecanoyl hydrazide	270	C16H34N2O	002619-88-7	22



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.120	4.0	ng	271390	1	7.944	1370780	20.0
n-Hexadecanoic ...	18.214	2.9	ng	743286	4	17.321	5166230	20.0
Nonadecyl penta...	21.234	3.5	ng	906473	5	21.587	5227330	20.0
1-Hexacosanol	23.919	2.5	ng	525453	6	24.765	4129440	20.0
unknown28.690	28.690	2.2	ng	463089	6	24.765	4129440	20.0