

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
 Data File : BG060219.D
 Acq On : 3 Jan 2024 8:40
 Operator : MA/JU
 Sample : 05909-13
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GHL-SS-51

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-BG122923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060219.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.113	3	4	13	rVB	418375	441932	5.30%	0.680%
2	5.041	327	332	336	rBV2	58703	93947	1.13%	0.145%
3	5.511	404	412	426	rBV	3059422	4997836	59.97%	7.691%
4	7.097	675	682	696	rBV	2975514	5224791	62.70%	8.041%
5	7.937	818	825	833	rBV	726127	1261263	15.14%	1.941%
6	9.101	1015	1023	1035	rBV	1675518	3059771	36.72%	4.709%
7	10.740	1295	1302	1316	rBV	1146166	2115660	25.39%	3.256%
8	13.196	1712	1720	1731	rBV	4742123	7458350	89.50%	11.478%
9	13.460	1759	1765	1774	rBV	269603	425213	5.10%	0.654%
10	14.576	1948	1955	1961	rBV	2361855	3578585	42.94%	5.507%
11	16.063	2201	2208	2222	rBV	4268745	6452199	77.43%	9.929%
12	17.320	2414	2422	2432	rBV	3001406	4597876	55.18%	7.076%
13	18.207	2569	2573	2581	rBV2	234487	382686	4.59%	0.589%
14	19.159	2727	2735	2738	rBV6	105447	185937	2.23%	0.286%
15	19.941	2862	2868	2878	rBV	6418242	8333228	100.00%	12.824%
16	20.164	2902	2906	2911	rBV4	74487	99598	1.20%	0.153%
17	20.264	2917	2923	2930	rVB3	154783	284969	3.42%	0.439%
18	20.446	2950	2954	2958	rBV2	159674	225900	2.71%	0.348%
19	21.239	3084	3089	3097	rBV2	513108	780204	9.36%	1.201%
20	21.521	3133	3137	3141	rBV	168992	228136	2.74%	0.351%
21	21.586	3141	3148	3160	rVV2	3387029	5640807	67.69%	8.681%
22	21.780	3177	3181	3185	rBV5	105696	196326	2.36%	0.302%
23	22.062	3226	3229	3238	rVB	99322	160582	1.93%	0.247%
24	22.150	3240	3244	3249	rVB	69908	116694	1.40%	0.180%
25	22.385	3278	3284	3288	rBV3	305267	704879	8.46%	1.085%
26	22.608	3317	3322	3328	rVB	223750	395978	4.75%	0.609%
27	22.673	3328	3333	3338	rBV2	102322	191729	2.30%	0.295%
28	23.061	3393	3399	3403	rBV5	54489	116459	1.40%	0.179%
29	23.860	3528	3535	3539	rBV2	278963	574920	6.90%	0.885%
30	23.913	3540	3544	3553	rVB3	242219	545640	6.55%	0.840%
31	24.764	3679	3689	3701	rBV	1597178	4554524	54.65%	7.009%
32	25.299	3777	3780	3788	rVB7	78335	167939	2.02%	0.258%
33	25.910	3875	3884	3891	rBV5	144448	429635	5.16%	0.661%
34	26.022	3897	3903	3911	rBV6	117259	353467	4.24%	0.544%
35	28.666	4346	4353	4368	rVB10	150168	603075	7.24%	0.928%

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ClientSampleId :
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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

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

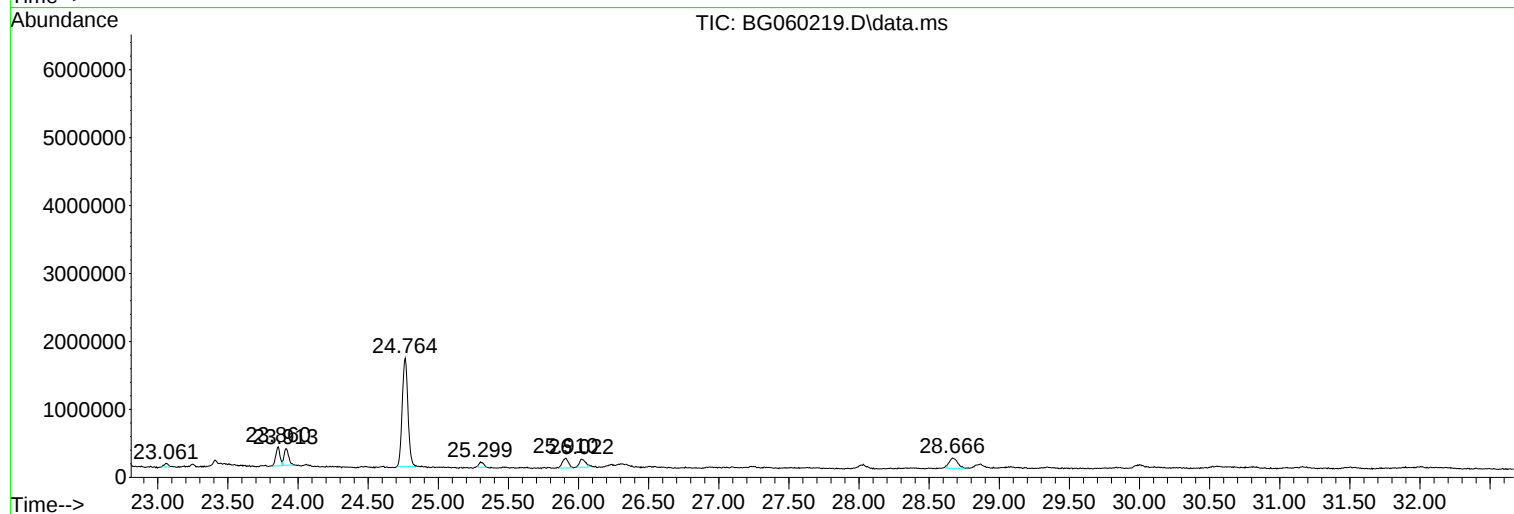
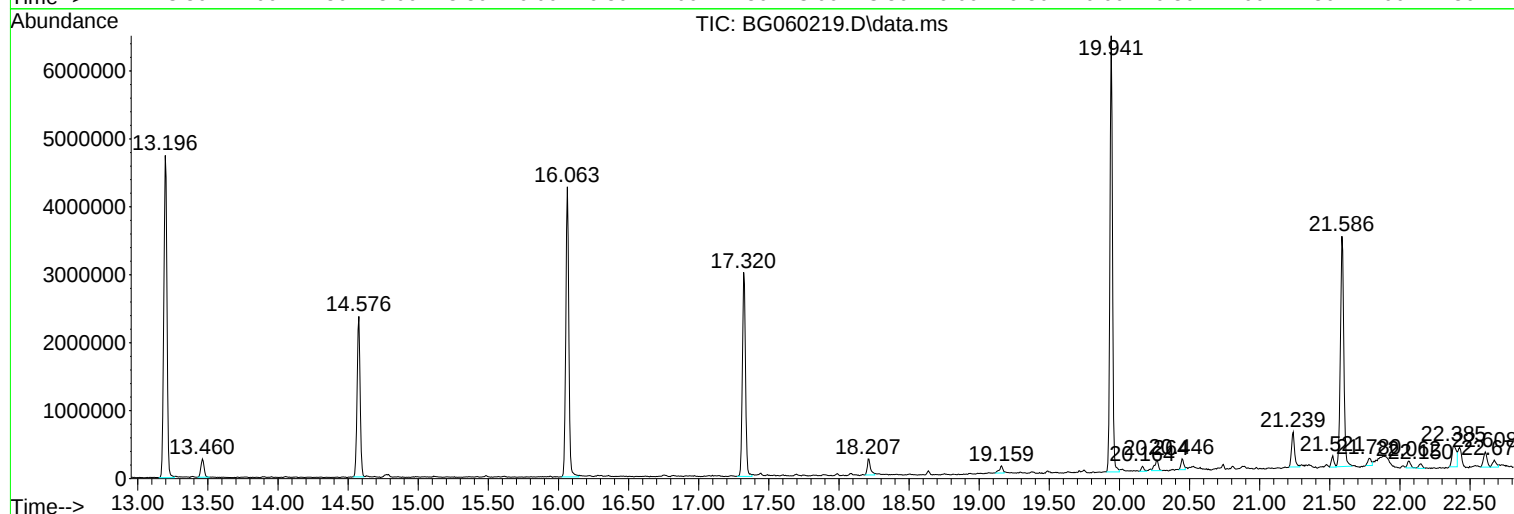
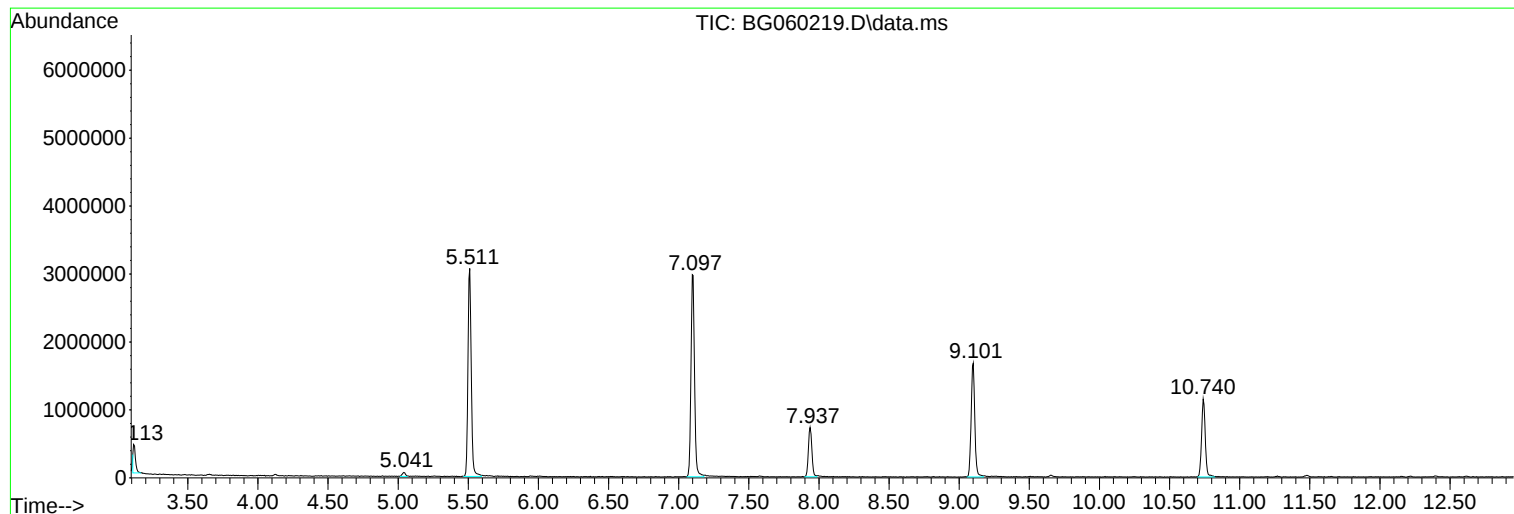
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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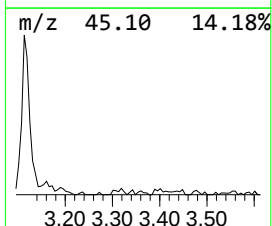
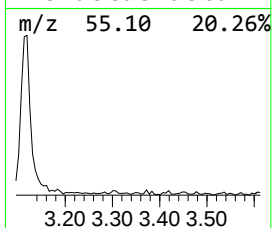
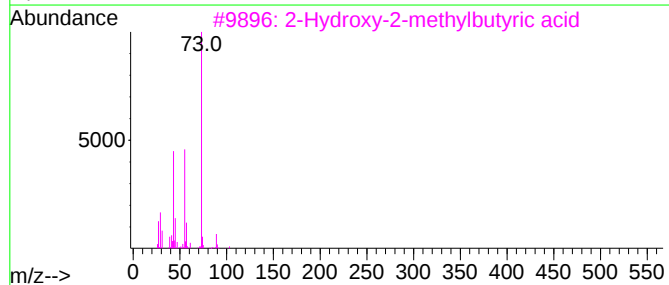
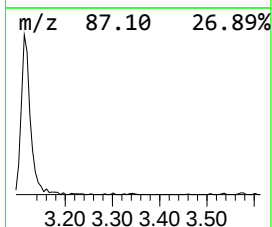
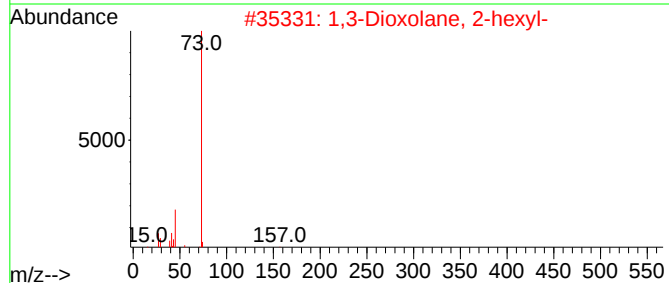
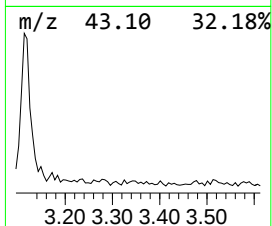
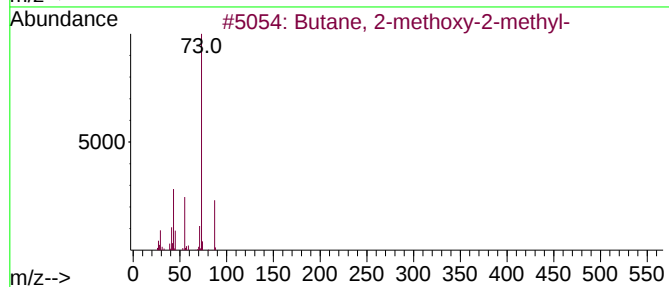
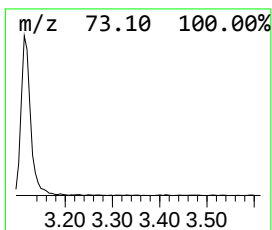
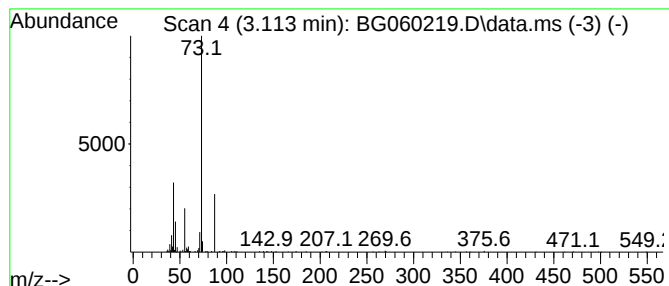
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.113	7.01 ng	441932	1,4-Dichlorobenzene-d4	7.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			1,3-Dioxolane, 2-hexyl-	158	C9H18O2	001708-34-5	12
3			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	12
4			1-Propene-1-thiol	74	C3H6S	000925-89-3	9
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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Instrument :
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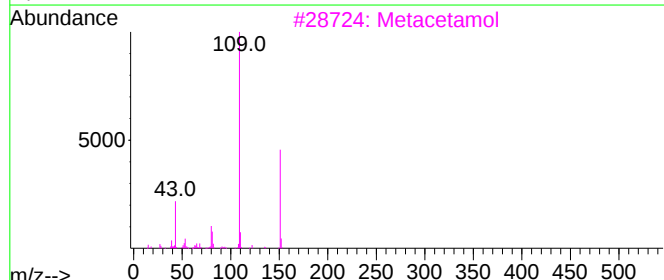
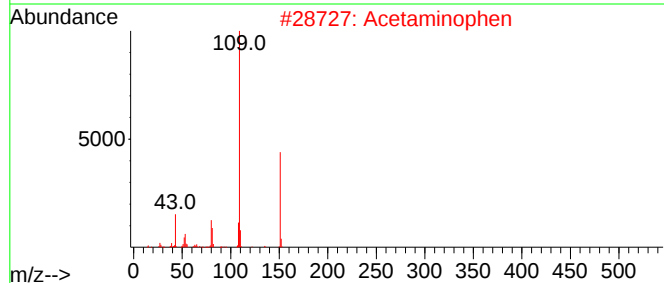
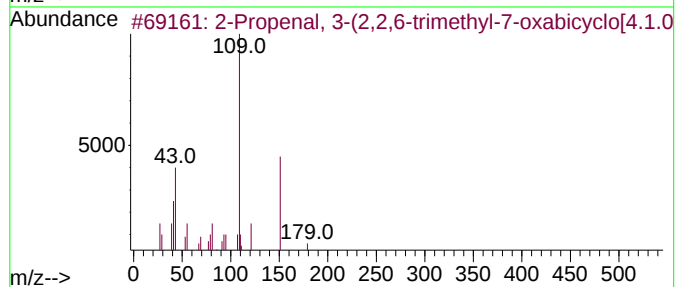
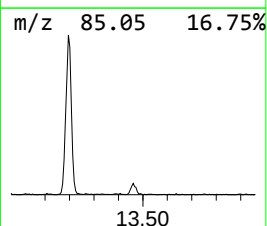
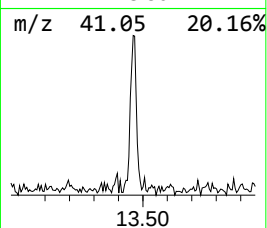
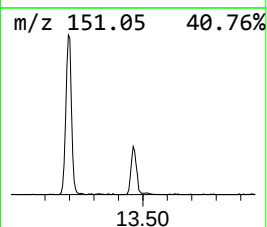
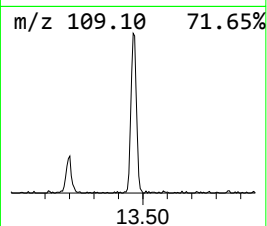
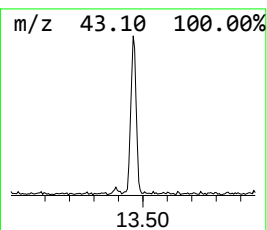
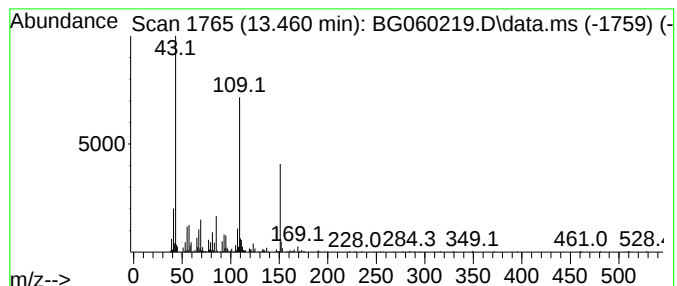
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Propenal, 3-(2,2,6-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.460	2.38 ng	425213	Acenaphthene-d10	14.576

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	64
2			Acetaminophen	151	C8H9NO2	000103-90-2	58
3			Metacetamol	151	C8H9NO2	000621-42-1	58
4			m-Isopropoxyaniline	151	C9H13NO	041406-00-2	58
5			Ethanone, 1-(4,5-diethyl-2-methy...	180	C12H20O	062338-24-3	47



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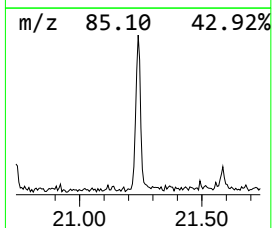
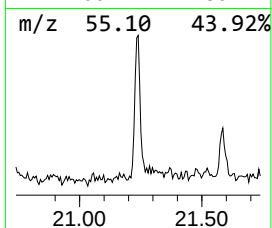
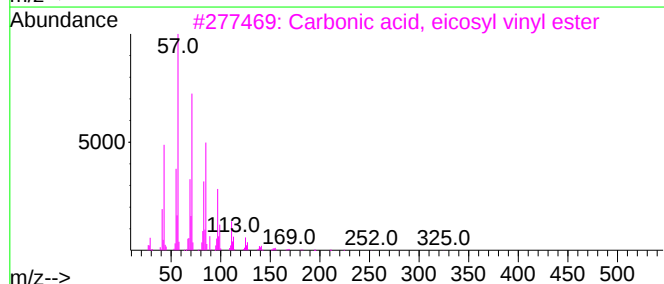
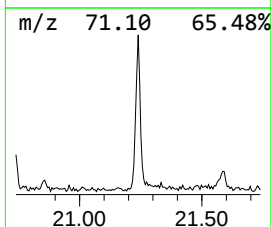
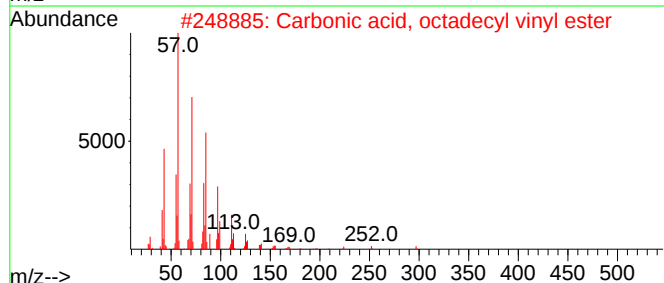
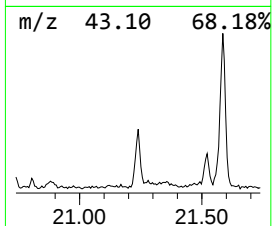
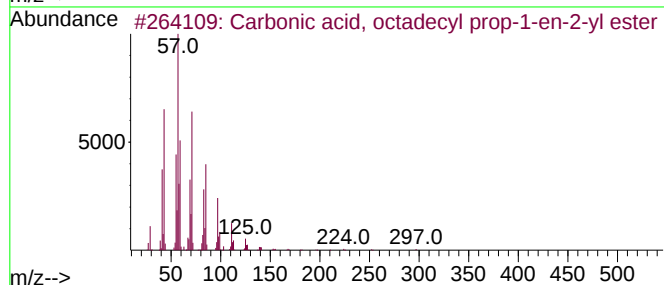
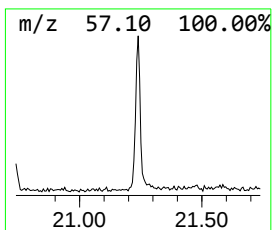
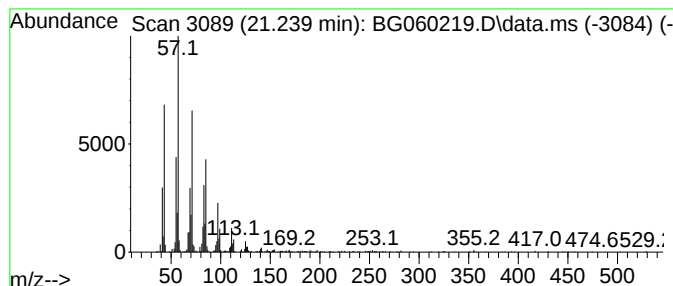
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Carbonic acid, octadecyl pr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.239	2.77 ng	780204	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
2			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	91
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	87
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	87
5			Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	74



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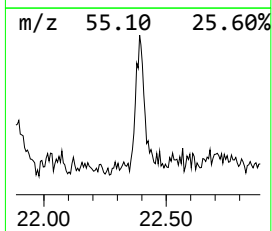
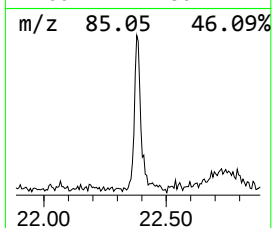
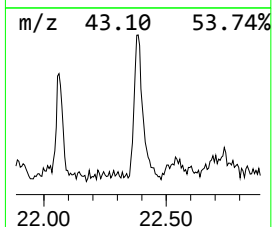
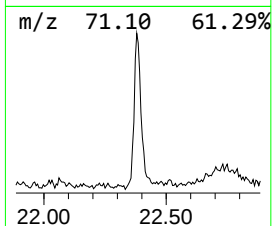
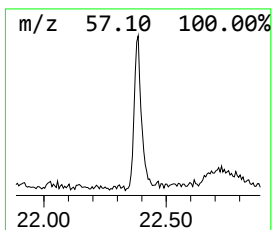
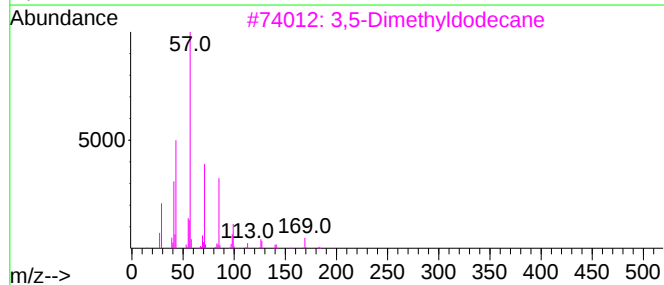
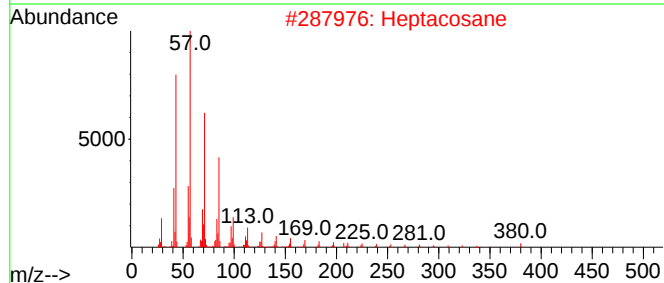
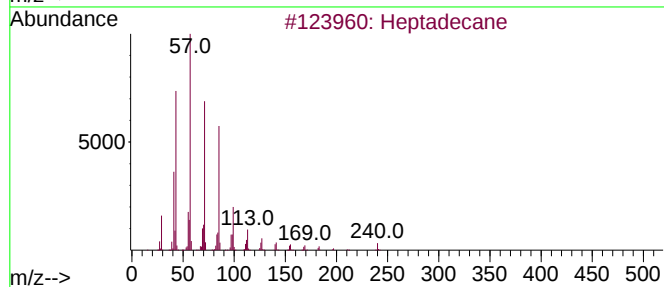
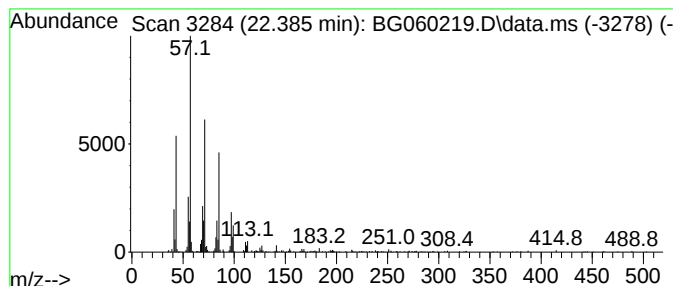
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.385	2.50 ng	704879	Chrysene-d12	21.586	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Heptacosane	380	C27H56	000593-49-7	86
3	3,5-Dimethyldodecane	198	C14H30	107770-99-0	80
4	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	80
5	1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	53



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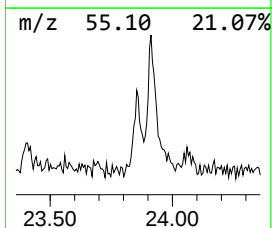
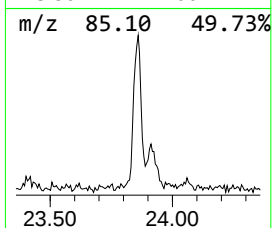
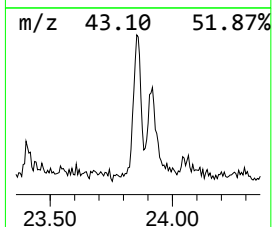
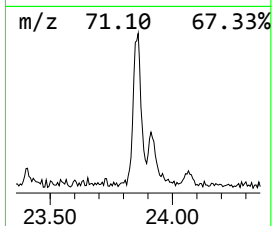
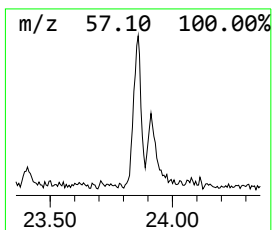
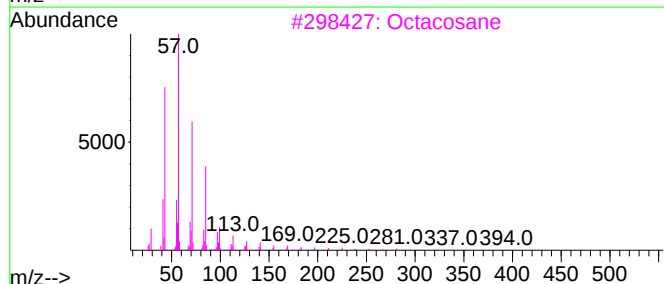
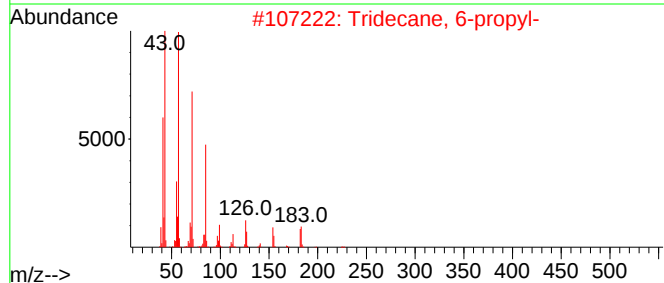
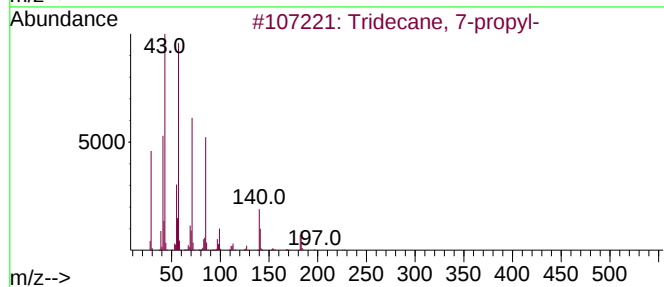
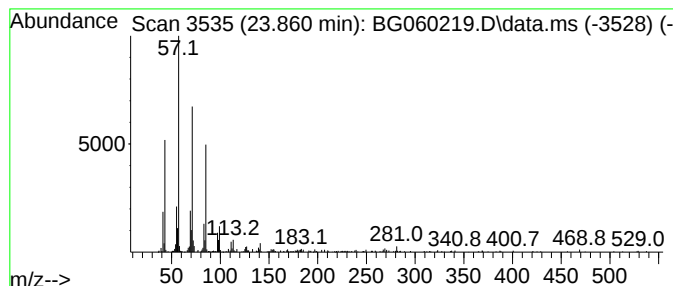
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tridecane, 7-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.860	2.52 ng	574920	Perylene-d12	24.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 7-propyl-	226	C16H34	055045-09-5	83
2			Tridecane, 6-propyl-	226	C16H34	055045-10-8	83
3			Octacosane	394	C28H58	000630-02-4	80
4			Docosane, 5-butyl-	366	C26H54	055282-16-1	80
5			Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060219.D
Acq On : 3 Jan 2024 8:40
Operator : MA/JU
Sample : 05909-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-51

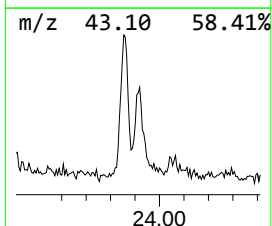
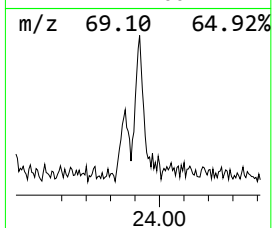
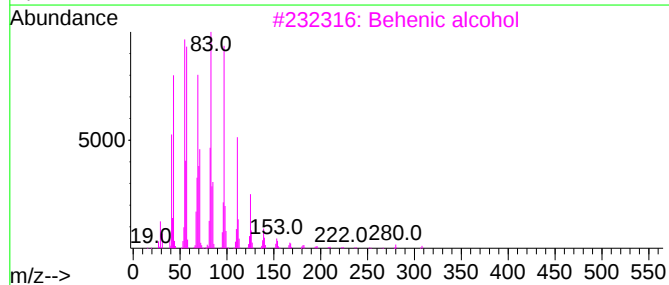
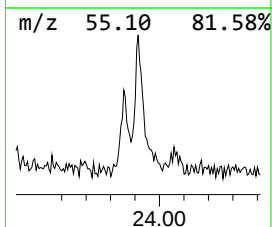
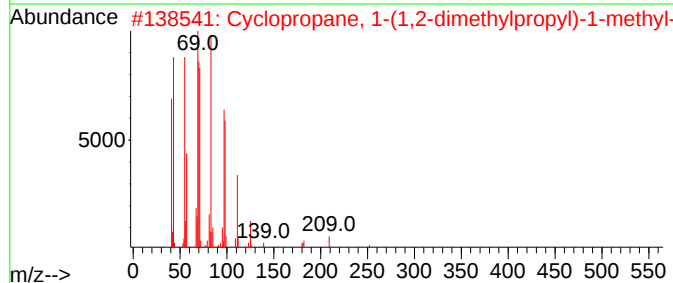
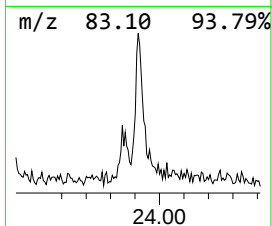
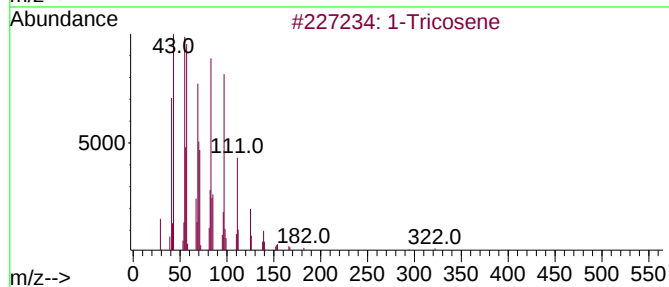
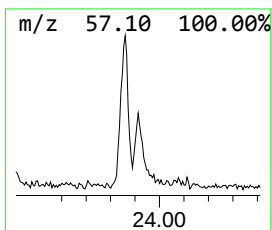
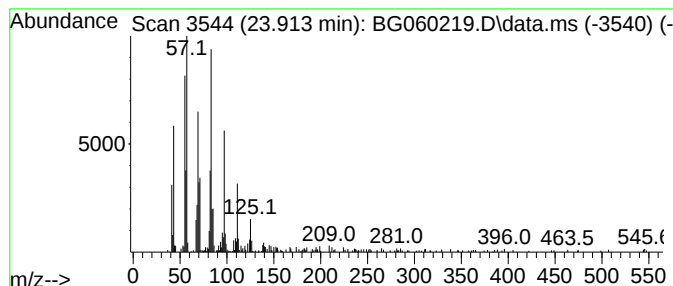
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Tricosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.913	2.40 ng	545640	Perylene-d12	24.759

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Tricosene	322	C23H46	018835-32-0	70
2		Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	68
3		Behenic alcohol	326	C22H46O	000661-19-8	62
4		1-Heneicosanol	312	C21H44O	015594-90-8	62
5		1-Heptacosanol	396	C27H56O	002004-39-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060219.D
Acq On : 3 Jan 2024 8:40
Operator : MA/JU
Sample : 05909-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

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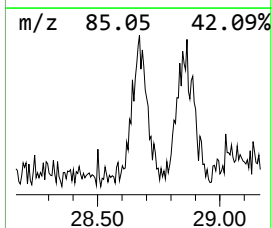
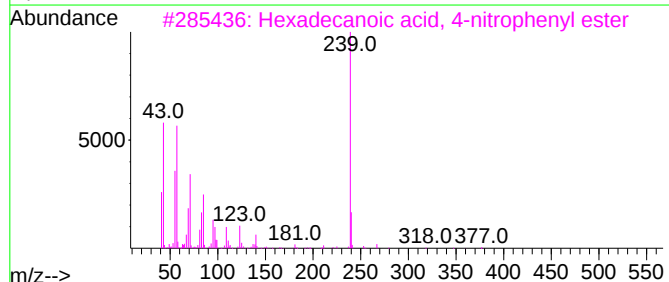
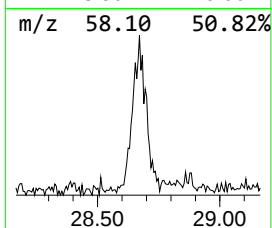
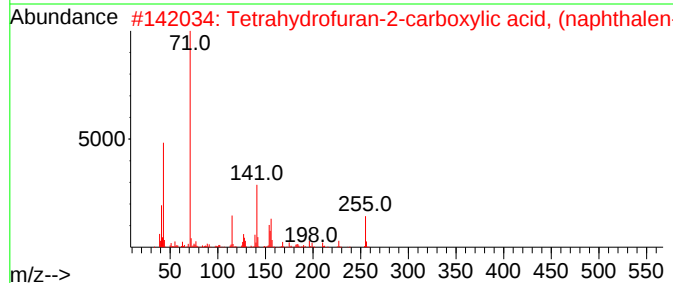
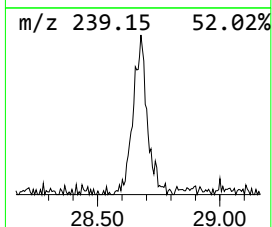
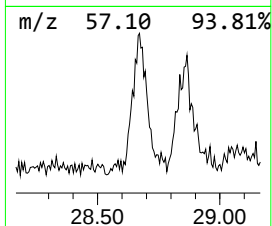
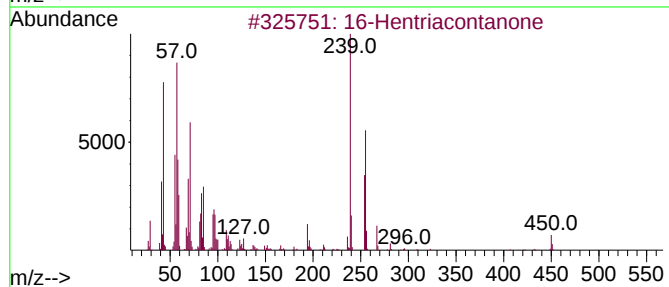
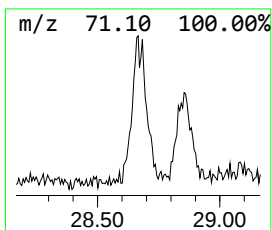
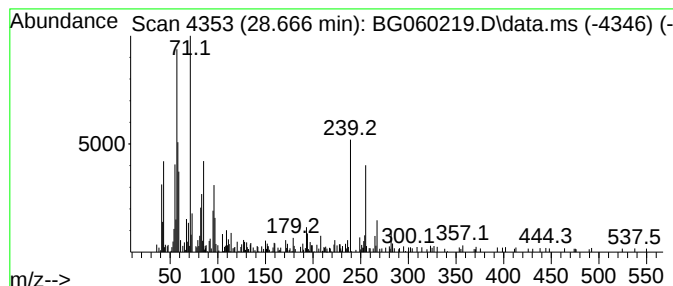
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 16-Hentriacontanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.666	2.65 ng	603075	Perylene-d12	24.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			16-Hentriacontanone	450	C31H62O	000502-73-8	53
2			Tetrahydrofuran-2-carboxylic aci...	255	C16H17NO2	1000317-13-3	35
3			Hexadecanoic acid, 4-nitrophenyl...	377	C22H35NO4	001492-30-4	32
4			24-.Xi.-methyl-5.alpha.-cholesta...	482	C28H50O6	1000103-51-9	25
5			9-Octadecene, 1,1-dimethoxy-, (Z)-	312	C20H40O2	015677-71-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060219.D
Acq On : 3 Jan 2024 8:40
Operator : MA/JU
Sample : 05909-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-51

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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
Butane, 2-metho...	3.113	7.0	ng	441932	1	7.937	1261260	20.0
2-Propenal, 3-(...	13.460	2.4	ng	425213	3	14.576	3578590	20.0
Carbonic acid, ...	21.239	2.8	ng	780204	5	21.586	5640810	20.0
Heptadecane	22.385	2.5	ng	704879	5	21.586	5640810	20.0
Tridecane, 7-pr...	23.860	2.5	ng	574920	6	24.759	4554520	20.0
1-Tricosene	23.913	2.4	ng	545640	6	24.759	4554520	20.0
16-Hentriaconta...	28.666	2.6	ng	603075	6	24.759	4554520	20.0