

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040524\
 Data File : BG060801.D
 Acq On : 5 Apr 2024 18:25
 Operator : MA/JU
 Sample : P1995-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 280648

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-BG032924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060801.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.182	27	33	46	rVB	274109	524416	7.43%	1.671%
2	5.538	427	434	446	rBV	984662	1550102	21.96%	4.939%
3	7.112	694	702	711	rBV	1011736	1738546	24.63%	5.539%
4	7.953	835	845	852	rBV	280468	467026	6.62%	1.488%
5	9.104	1033	1041	1052	rBV	608765	1097877	15.55%	3.498%
6	10.749	1312	1321	1330	rBV	362484	649615	9.20%	2.070%
7	13.205	1732	1739	1748	rBV	1381038	2217613	31.41%	7.066%
8	13.381	1765	1769	1781	rBV6	48981	107820	1.53%	0.344%
9	14.016	1873	1877	1882	rBV	294996	441024	6.25%	1.405%
10	14.134	1893	1897	1905	rVB4	132070	243171	3.44%	0.775%
11	14.339	1927	1932	1939	rBV8	165786	474345	6.72%	1.511%
12	14.427	1942	1947	1954	rVB	479778	797488	11.30%	2.541%
13	14.498	1955	1959	1964	rBV5	140632	281418	3.99%	0.897%
14	14.580	1966	1973	1978	rBV2	628450	1356129	19.21%	4.321%
15	15.385	2106	2110	2116	rVB2	681270	993995	14.08%	3.167%
16	16.072	2223	2227	2232	rBV	1247732	1801352	25.52%	5.739%
17	19.333	2778	2782	2788	rVB	1864636	2306617	32.68%	7.349%
18	19.956	2884	2888	2902	rVB	2290284	3263637	46.23%	10.398%
19	21.272	3109	3112	3118	rVB3	189261	291826	4.13%	0.930%
20	21.525	3149	3155	3160	rVB	5051599	7059149	100.00%	22.491%
21	21.595	3161	3167	3172	rVV2	658638	1120105	15.87%	3.569%
22	22.447	3308	3312	3317	rBV3	109842	174425	2.47%	0.556%
23	23.317	3454	3460	3469	rVB	289346	548439	7.77%	1.747%
24	23.740	3528	3532	3540	rBV2	70728	164759	2.33%	0.525%
25	23.934	3559	3565	3570	rBV	142624	300069	4.25%	0.956%
26	24.580	3670	3675	3683	rVB	78304	204509	2.90%	0.652%
27	24.733	3692	3701	3712	rBV	437073	1210637	17.15%	3.857%

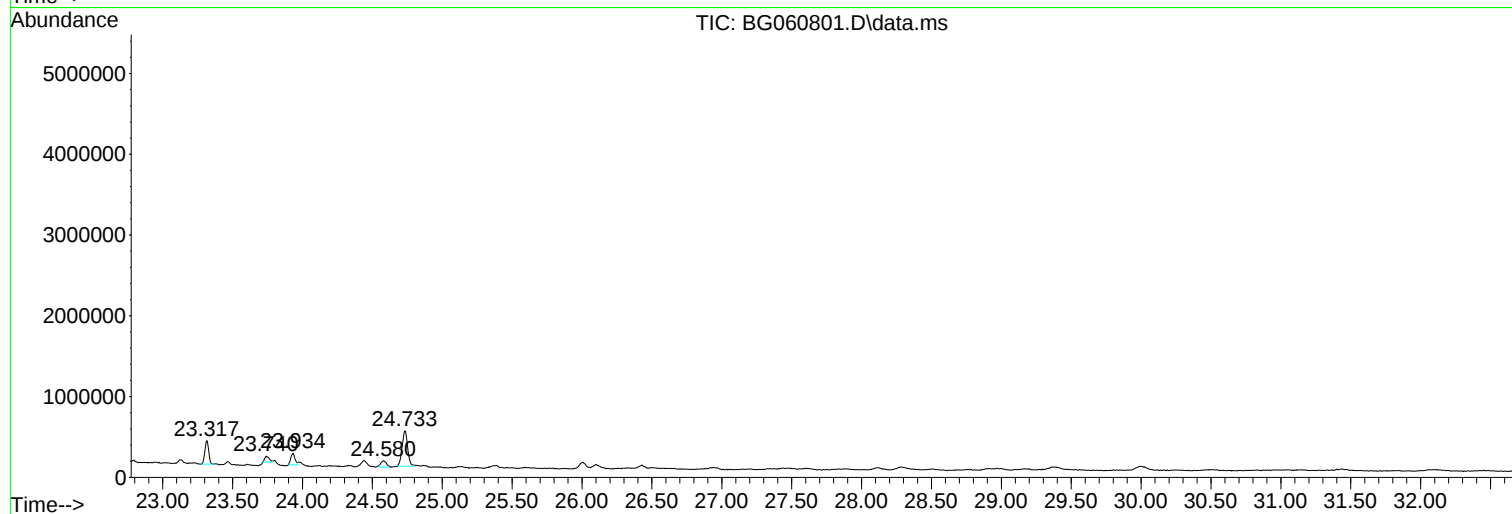
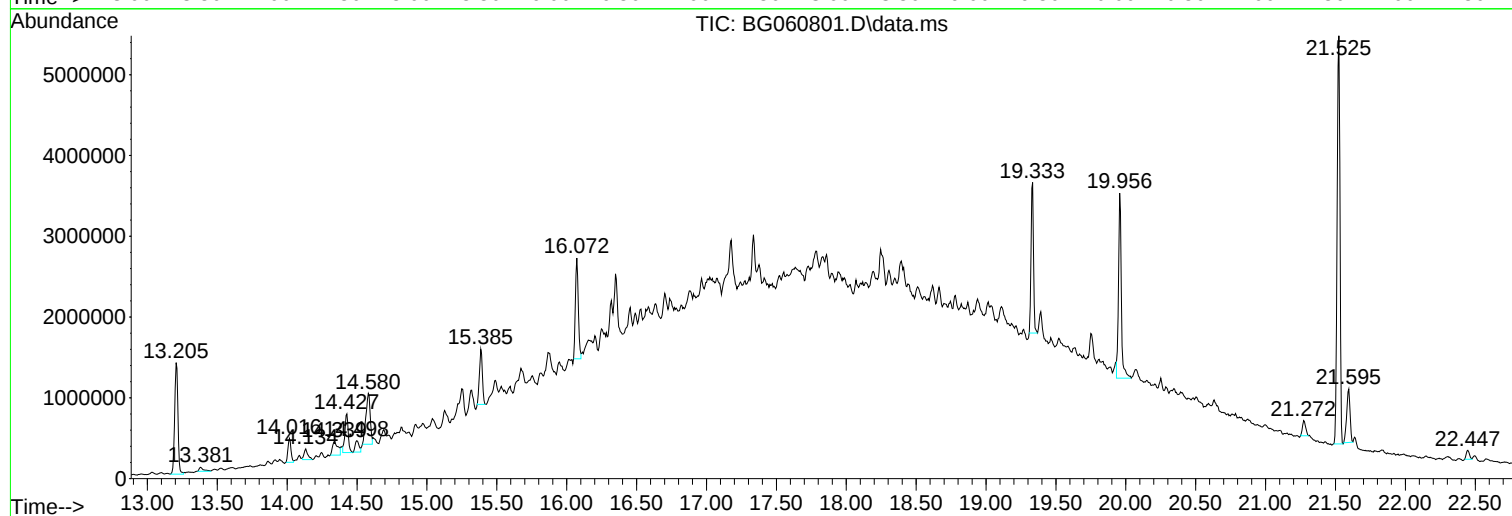
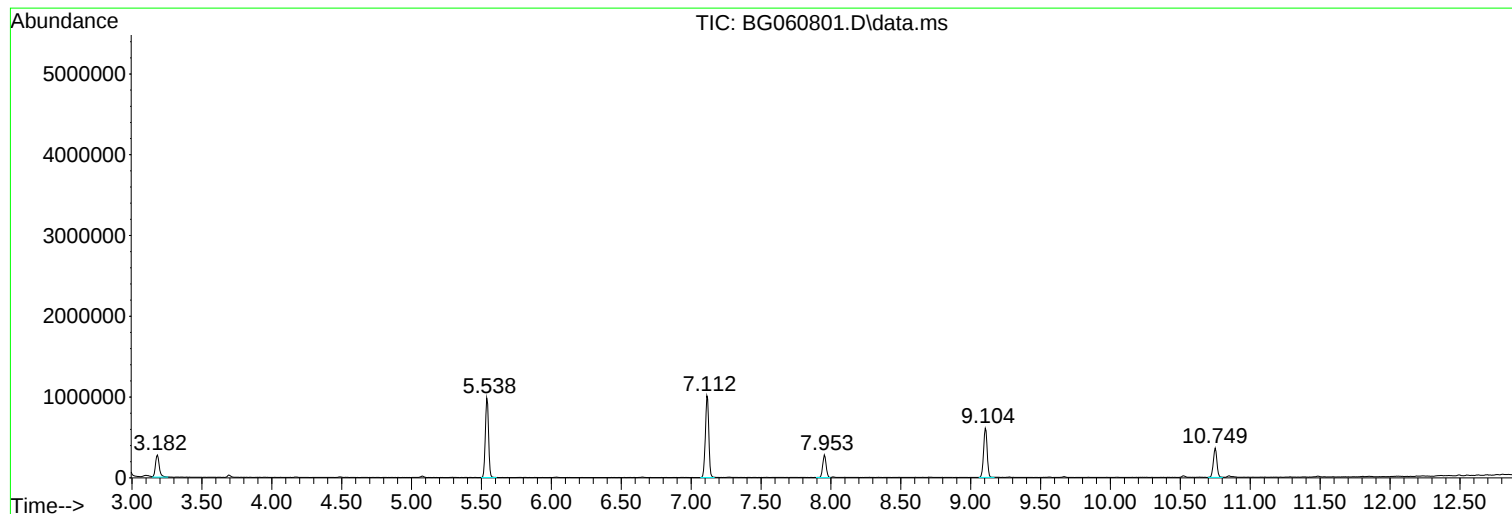
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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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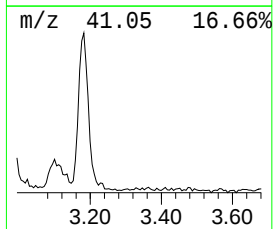
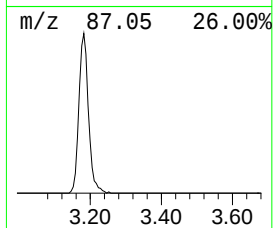
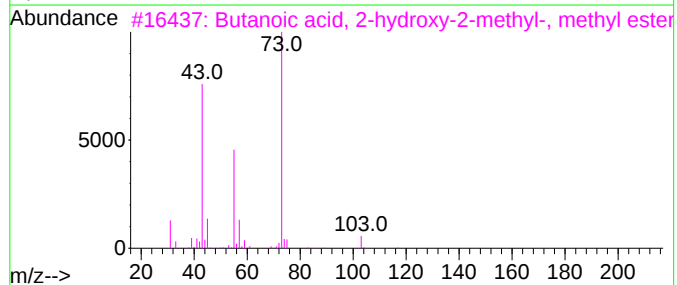
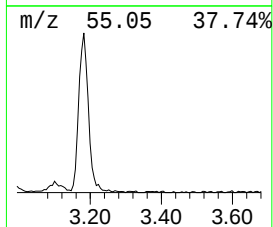
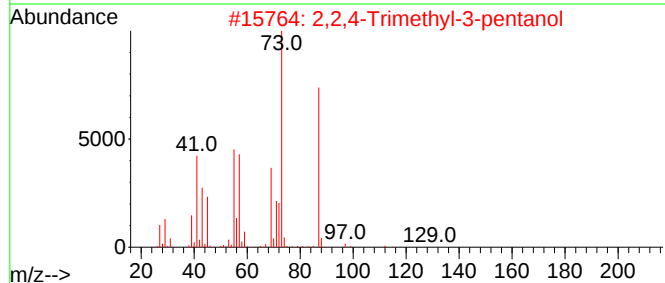
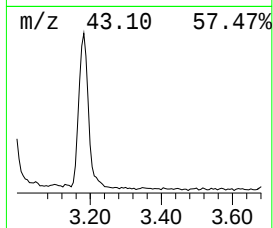
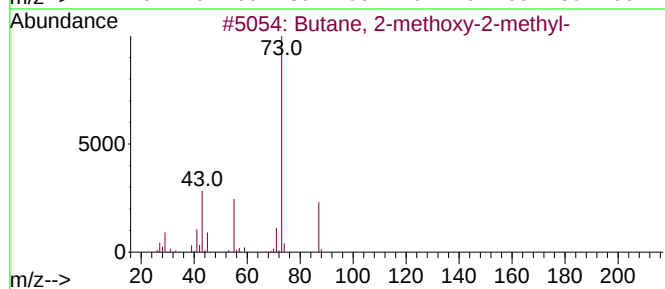
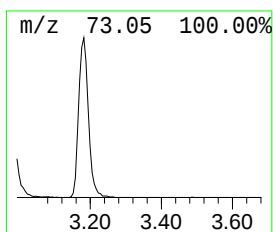
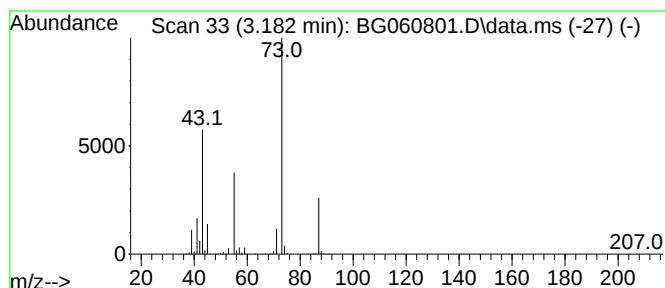
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.182	22.46 ng	524416	1,4-Dichlorobenzene-d4	7.952

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Butanoic acid, 2-hydroxy-2-methyl...	132	C6H12O3	032793-34-3	38
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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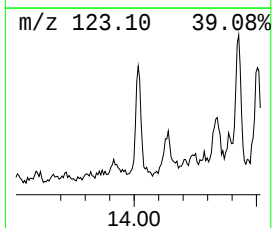
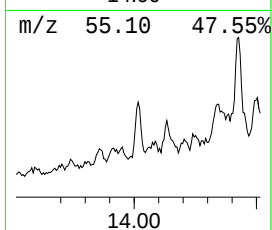
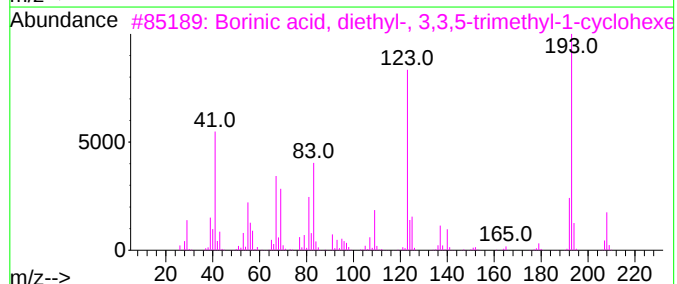
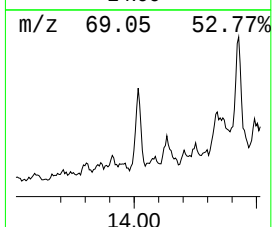
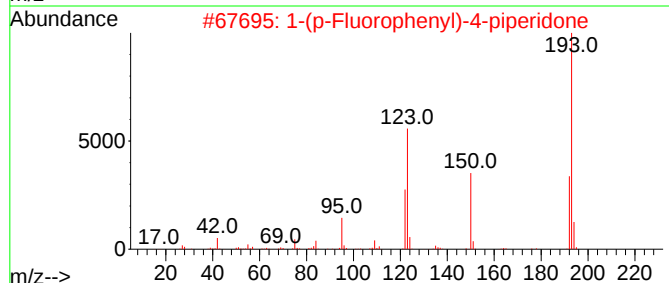
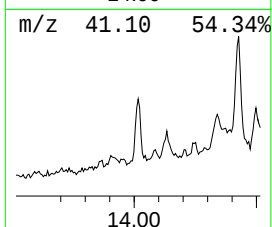
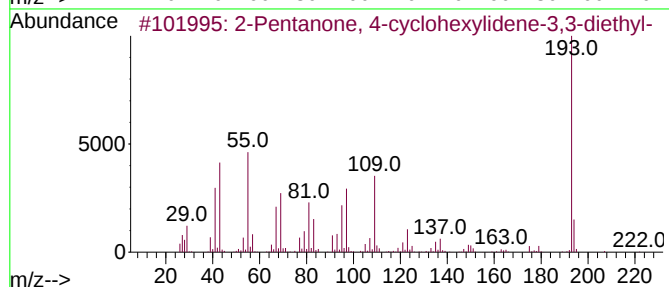
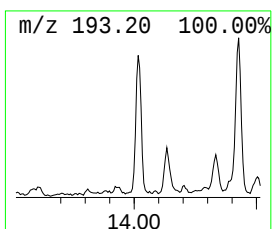
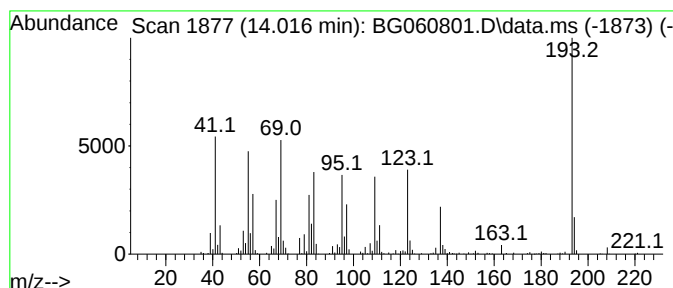
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-cyclohexylid... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.016	6.50 ng	441024	Acenaphthene-d10			14.580
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...		222	C15H26O	313253-65-5	50
2	1-(p-Fluorophenyl)-4-piperidone		193	C11H12FNO	1000238-56-7	46
3	Borinic acid, diethyl-, 3,3,5-tr...		208	C13H25BO	057387-76-5	32
4	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	30
5	2-Anthracenamine		193	C14H11N	000613-13-8	27



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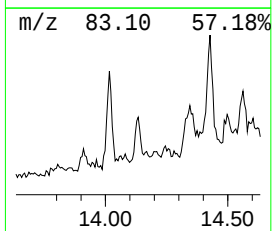
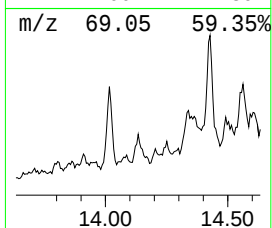
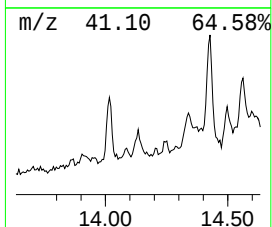
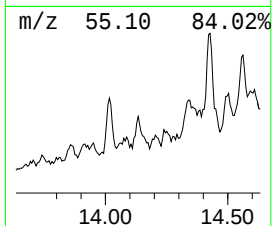
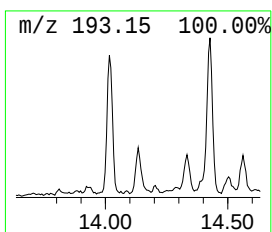
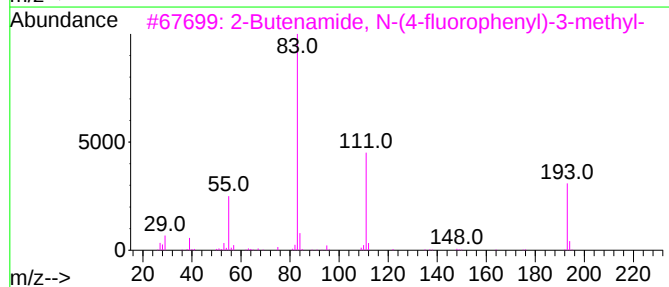
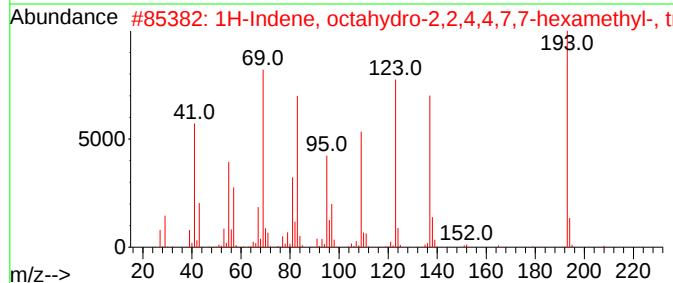
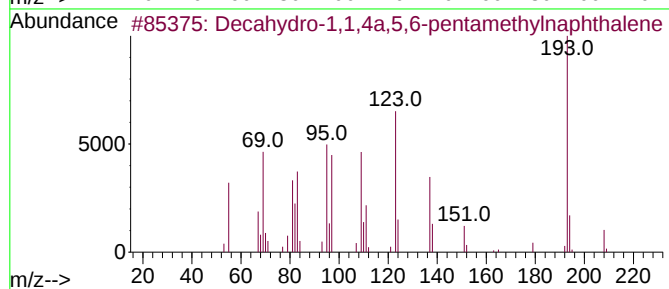
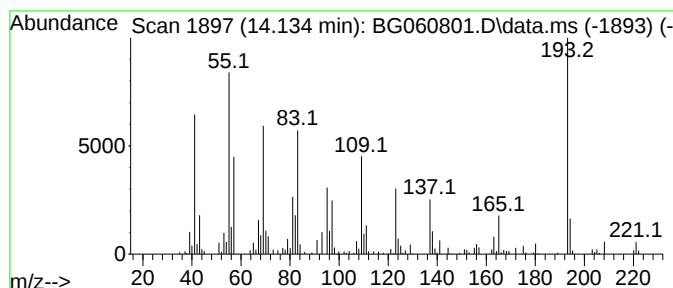
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.134	3.59 ng	243171	Acenaphthene-d10	14.580	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	55
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	53
3	2-Butenamide, N-(4-fluorophenyl)...	193	C11H12FNO	1000307-26-7	43
4	2-Anthracenamine	193	C14H11N	000613-13-8	35
5	1-Anthracenamine	193	C14H11N	000610-49-1	35



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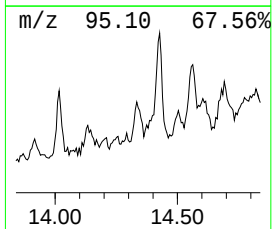
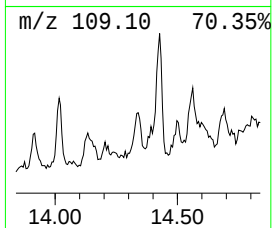
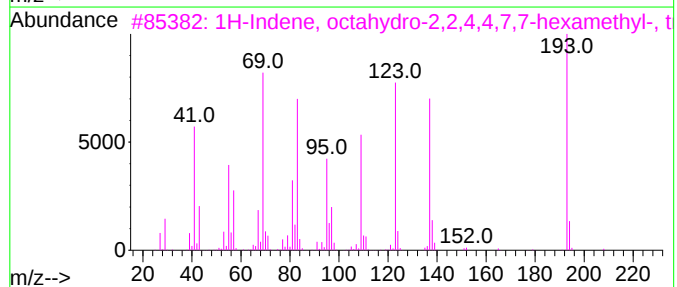
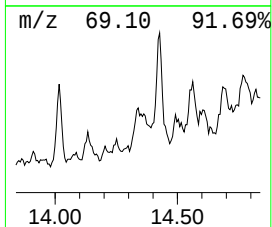
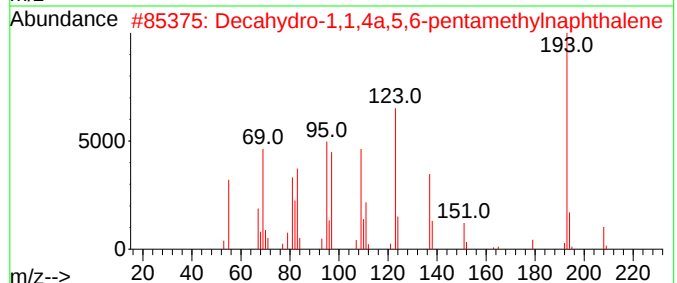
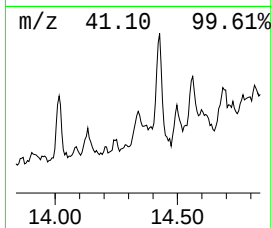
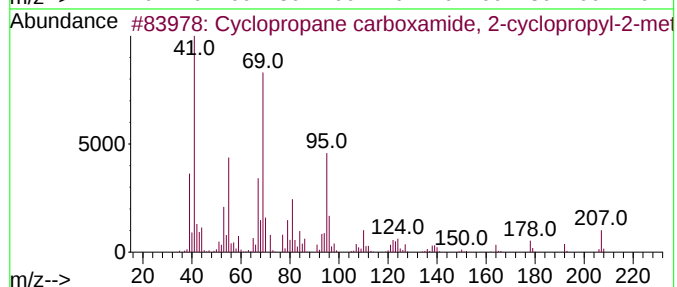
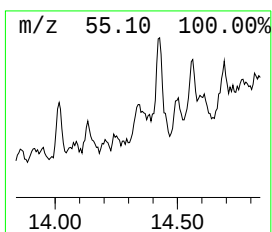
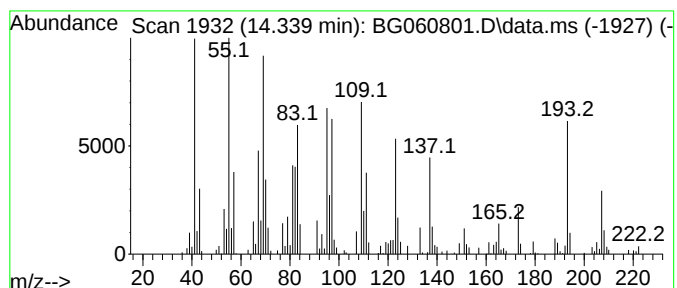
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.339 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.339	7.00 ng	474345	Acenaphthene-d10	14.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	42
2			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	41
3			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
4			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	35
5			Phosphinecarboxylic acid, dietho...	210	C7H15O5P	001474-78-8	25



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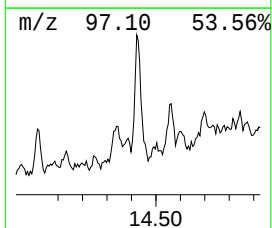
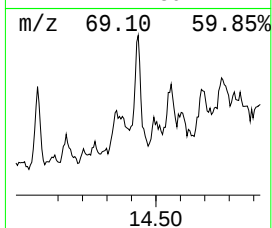
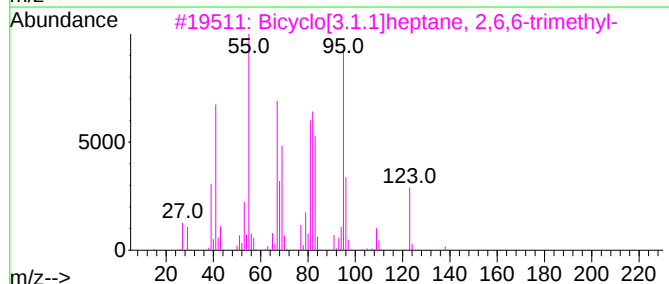
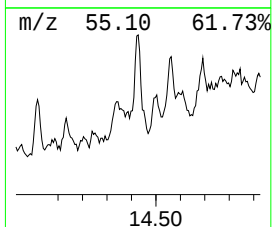
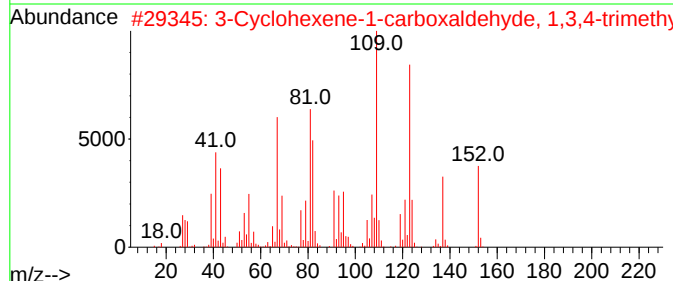
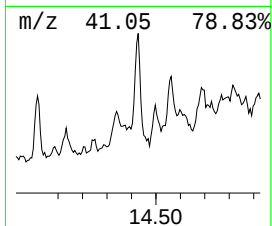
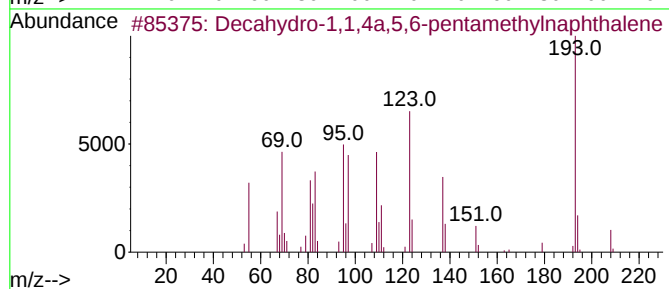
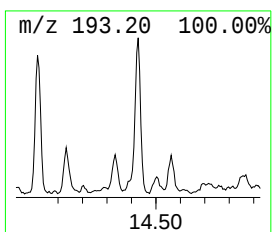
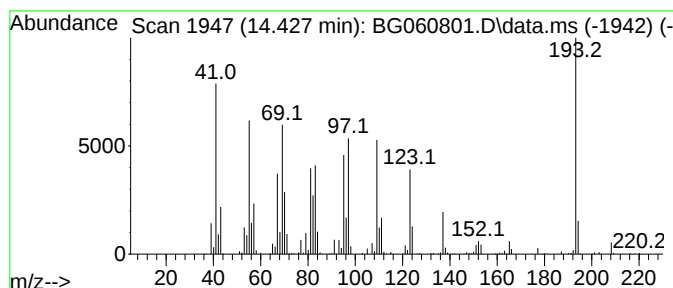
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown14.427 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.427	11.76 ng	797488	Acenaphthene-d10	14.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	49
2			3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	22
3			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	20
4			Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	15
5			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	15



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280648

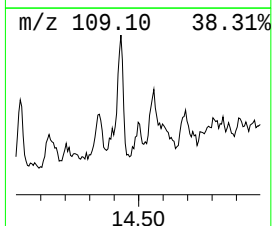
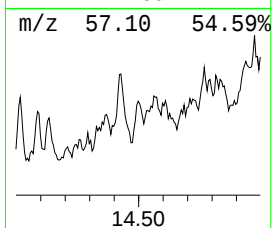
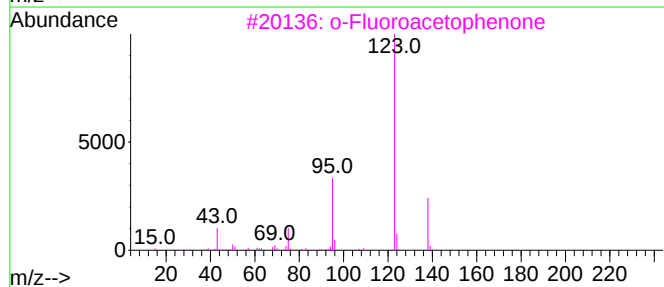
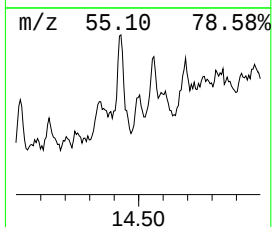
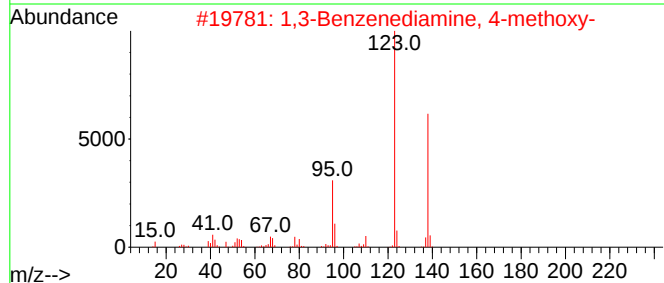
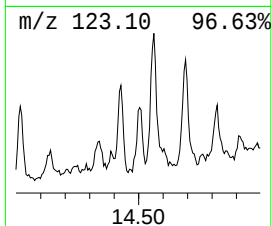
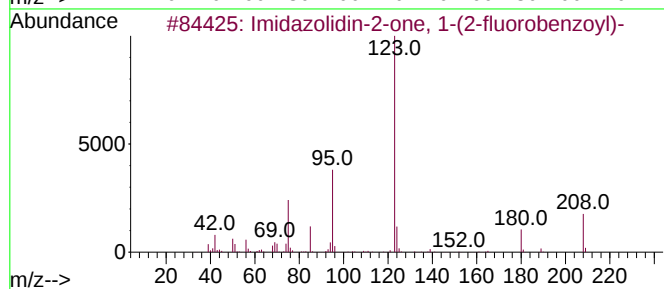
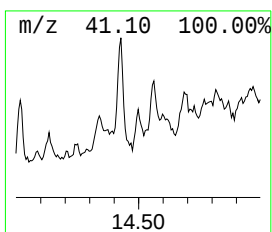
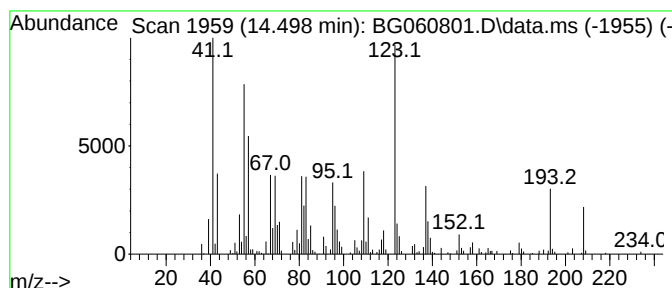
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.498 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	4.15 ng	281418	Acenaphthene-d10	14.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Imidazolidin-2-one, 1-(2-fluorobenzoyl)-	208	C10H9FN2O2	1010310-62-2	43
2			1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	38
3			o-Fluoroacetophenone	138	C8H7FO	000445-27-2	38
4			2'-Fluoropropiophenone	152	C9H9FO	000446-22-0	35
5			1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	051504-54-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040524\
Data File : BG060801.D
Acq On : 5 Apr 2024 18:25
Operator : MA/JU
Sample : P1995-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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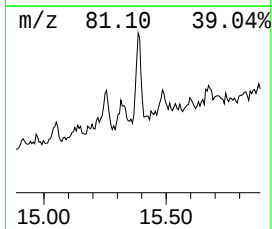
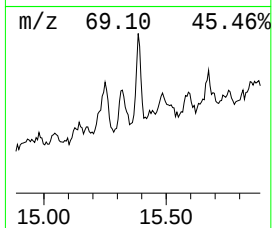
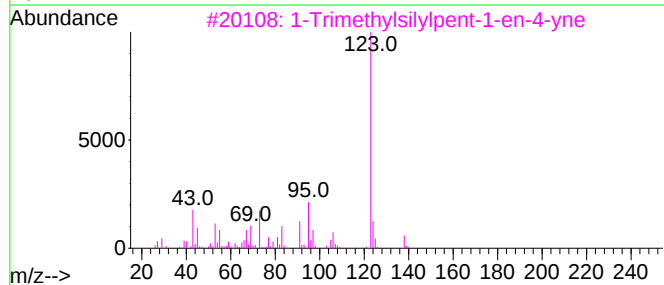
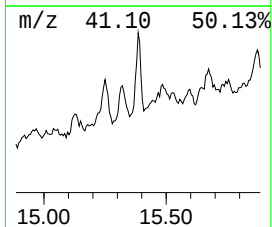
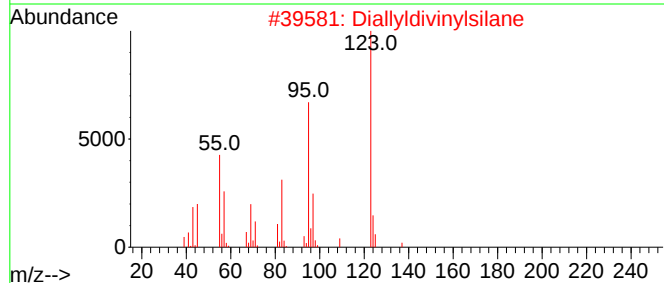
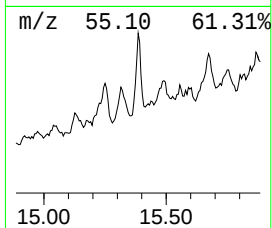
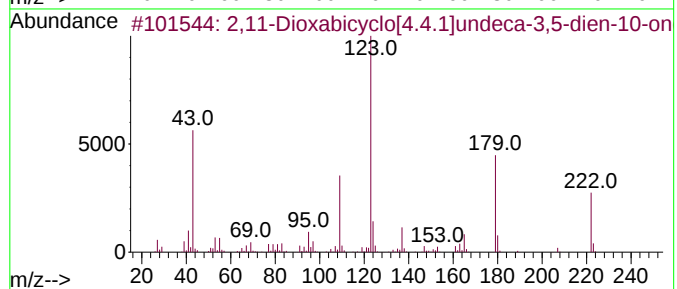
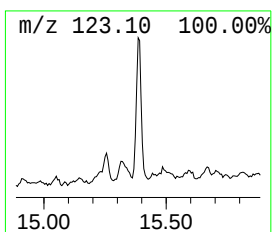
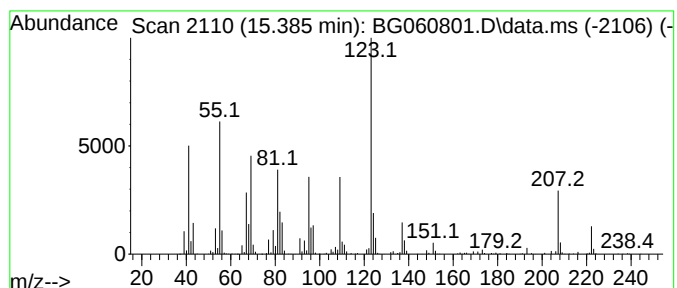
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TIC Integration Parameters: LSCINT.P

Peak Number 7 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.385	14.66 ng	993995	Acenaphthene-d10	14.580

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	59
2		Diallyldivinylsilane	164	C10H16Si	119901-88-1	50
3		1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	50
4		1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	47
5		Phorone	138	C9H14O	000504-20-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040524\
Data File : BG060801.D
Acq On : 5 Apr 2024 18:25
Operator : MA/JU
Sample : P1995-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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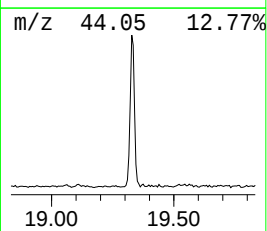
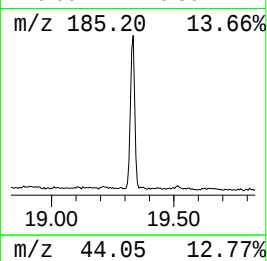
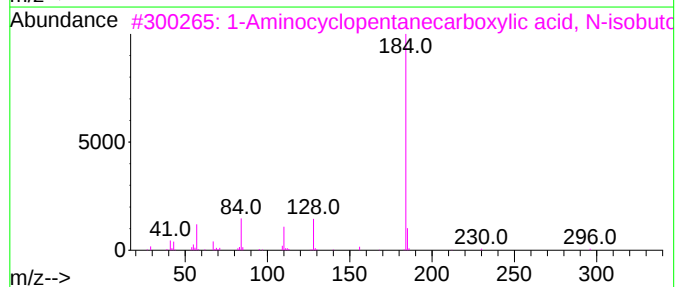
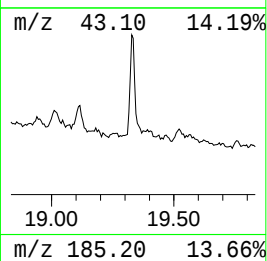
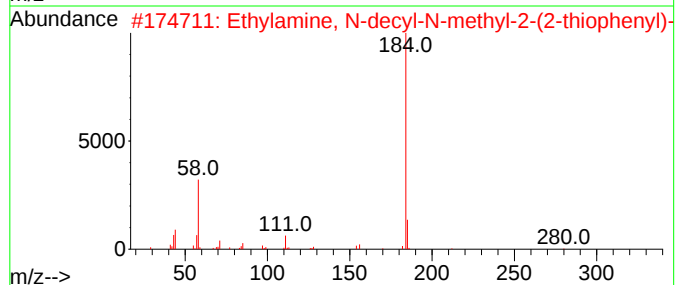
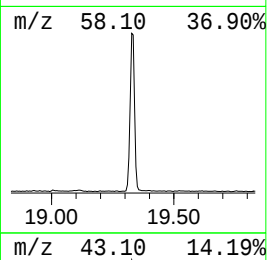
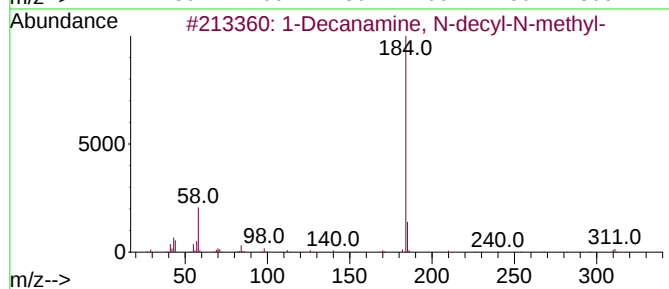
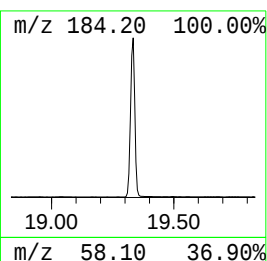
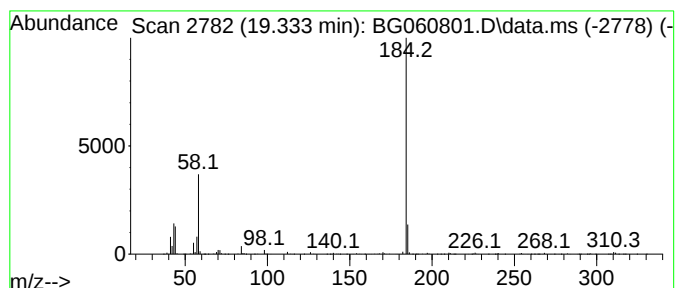
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Decanamine, N-decyl-N-met... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.333	25.61 ng	2306620	Phenanthrene-d10	17.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decanamine, N-decyl-N-methyl-	311	C21H45N	007396-58-9	72
2			Ethylamine, N-decyl-N-methyl-2-(...	281	C17H31NS	1000310-34-4	72
3			1-Aminocyclopentanecarboxylic ac...	397	C23H43NO4	1000329-10-8	53
4			1-Aminocyclopentanecarboxylic ac...	425	C25H47NO4	1000329-10-9	53
5			1-Aminocyclopentanecarboxylic ac...	313	C17H31NO4	1000329-09-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040524\
Data File : BG060801.D
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Sample : P1995-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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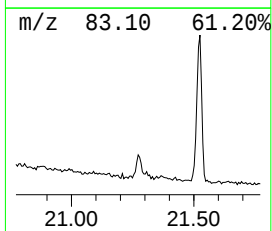
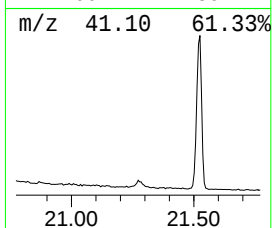
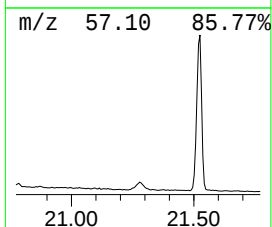
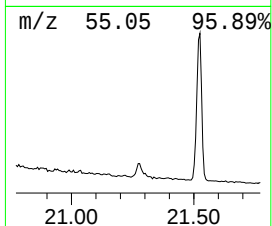
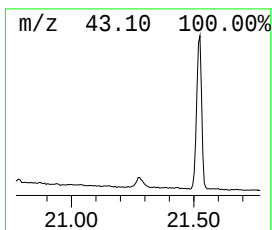
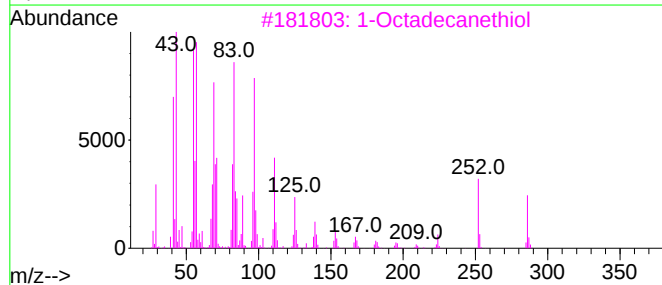
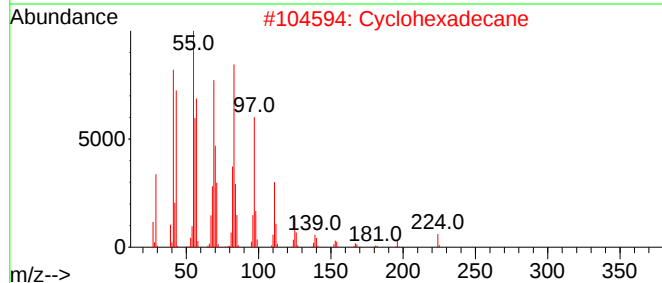
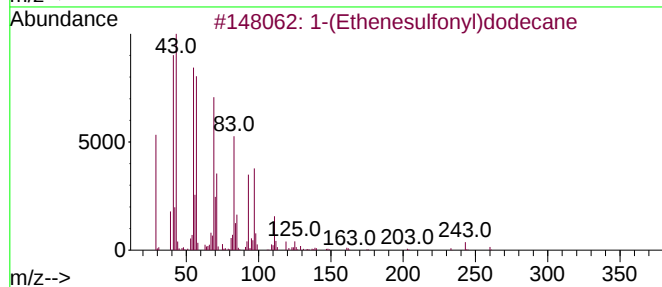
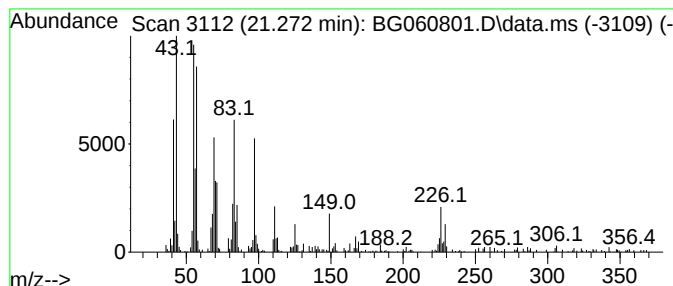
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 1-(Ethenesulfonyl)dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.272	5.21 ng	291826	Chrysene-d12		21.595	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-(Ethenesulfonyl)dodecane		260	C14H28O2S	030719-66-5	89
2	Cyclohexadecane		224	C16H32	000295-65-8	86
3	1-Octadecanethiol		286	C18H38S	002885-00-9	86
4	1-Hexacosene		364	C26H52	018835-33-1	76
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040524\
Data File : BG060801.D
Acq On : 5 Apr 2024 18:25
Operator : MA/JU
Sample : P1995-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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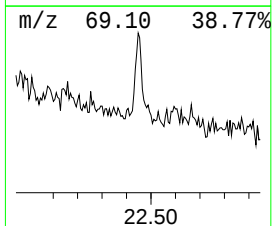
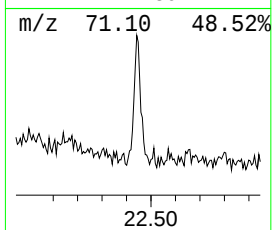
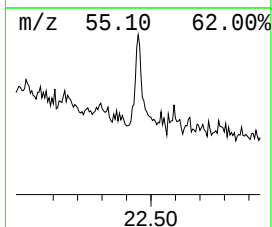
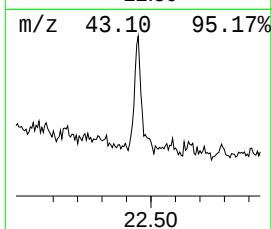
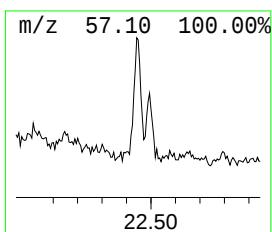
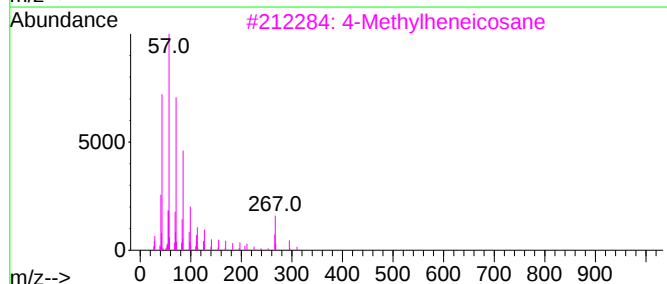
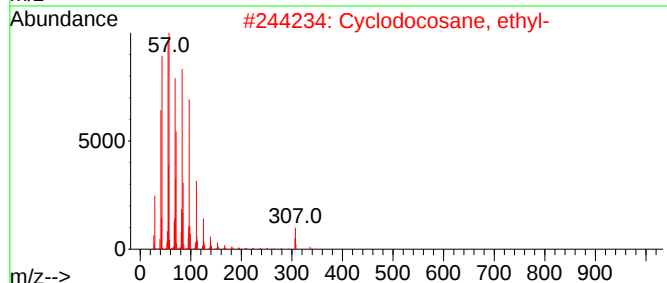
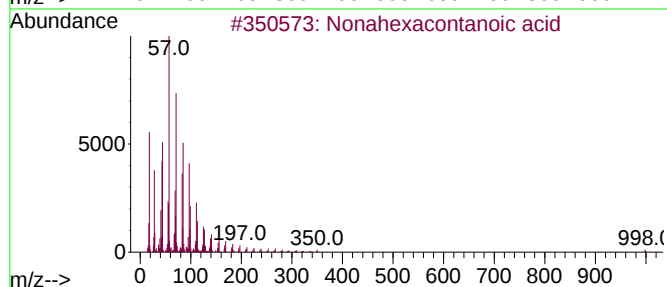
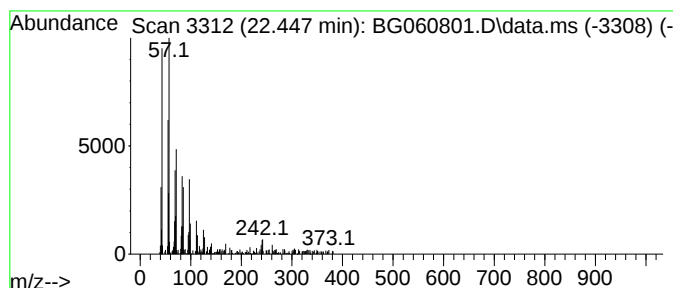
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonaheptacontanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.447	3.11 ng	174425	Chrysene-d12	21.595

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonaheptacontanoic acid	999	C69H138O2	040710-32-5	87
2		Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	70
3		4-Methylheneicosane	310	C22H46	025117-29-7	64
4		Z-5-Nonadecene	266	C19H38	1000131-11-8	62
5		Eicosane	282	C20H42	000112-95-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040524\
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Sample : P1995-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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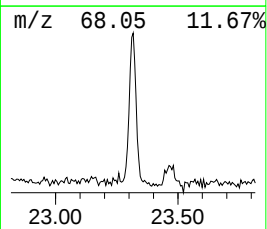
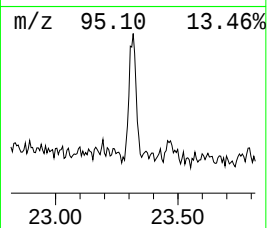
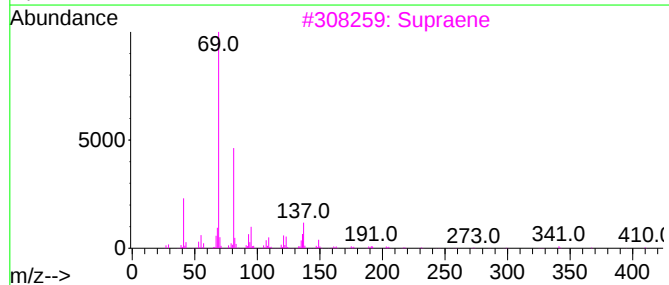
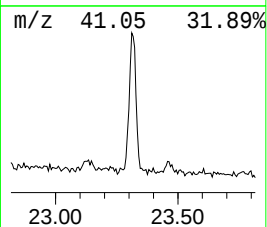
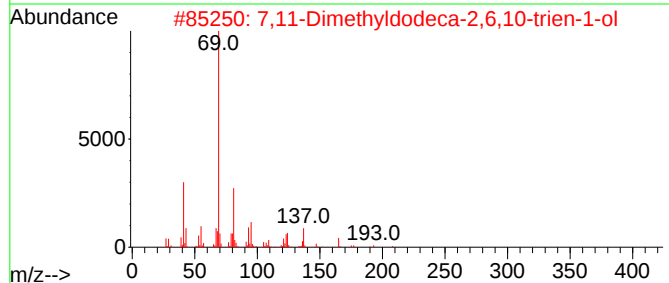
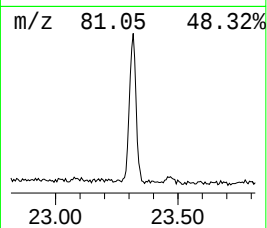
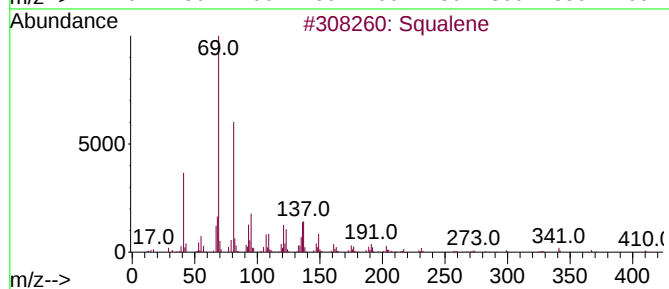
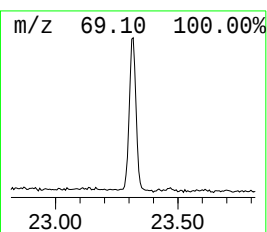
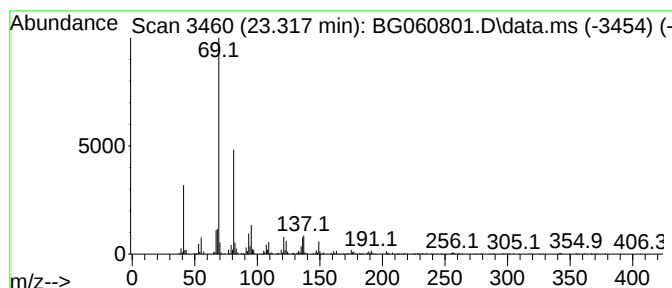
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.317	9.06 ng	548439	Perylene-d12	24.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	87
3			Supraene	410	C30H50	007683-64-9	87
4			trans-Farnesol	222	C15H26O	000106-28-5	72
5			Bis(3-methylbut-3-enyl) phthalate	302	C18H22O4	022711-53-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040524\
Data File : BG060801.D
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Sample : P1995-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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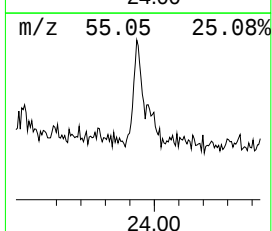
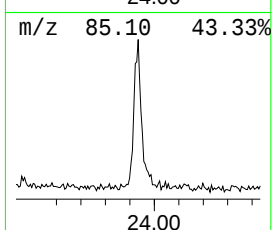
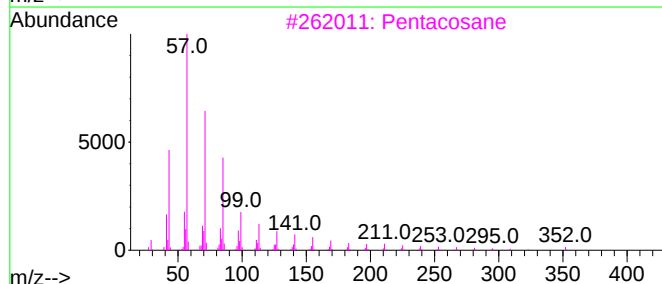
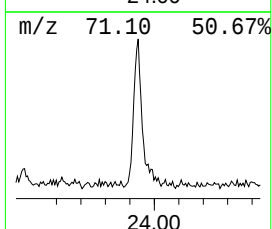
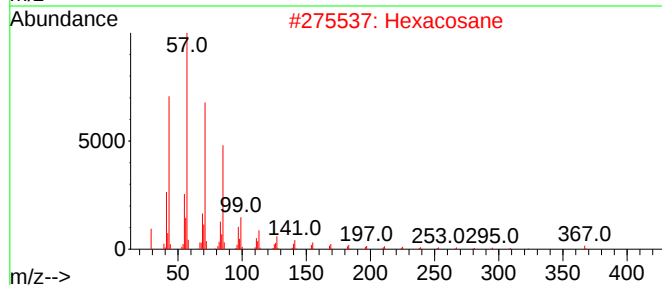
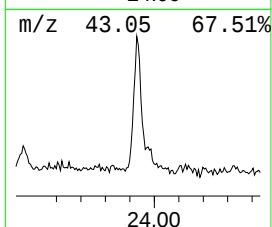
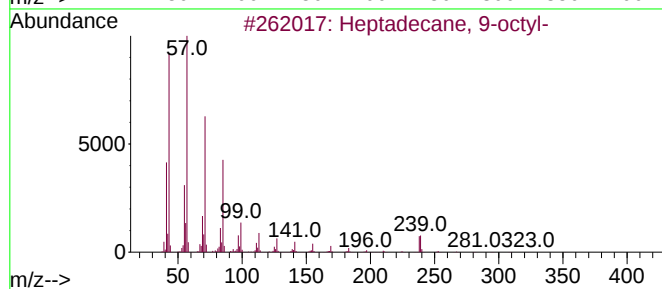
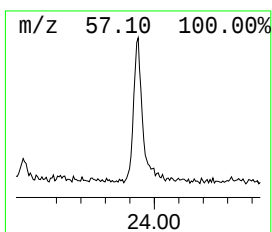
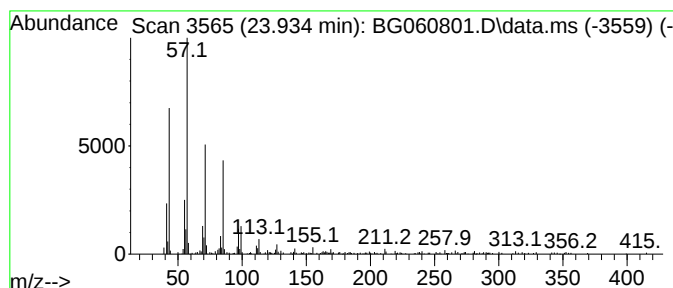
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.934	4.96 ng	300069	Perylene-d12	24.733

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
2		Hexacosane	366	C26H54	000630-01-3	86
3		Pentacosane	352	C25H52	000629-99-2	83
4		Undecane, 3-methyl-	170	C12H26	001002-43-3	80
5		Tetracosane	338	C24H50	000646-31-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040524\
Data File : BG060801.D
Acq On : 5 Apr 2024 18:25
Operator : MA/JU
Sample : P1995-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
280648

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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...	3.182	22.5	ng	524416	1	7.952	467026	20.0
2-Pentanone, 4-...	14.016	6.5	ng	441024	3	14.580	1356130	20.0
Decahydro-1,1,4...	14.134	3.6	ng	243171	3	14.580	1356130	20.0
unknown14.339	14.339	7.0	ng	474345	3	14.580	1356130	20.0
unknown14.427	14.427	11.8	ng	797488	3	14.580	1356130	20.0
unknown14.498	14.498	4.2	ng	281418	3	14.580	1356130	20.0
2,11-Dioxabicyc...	15.385	14.7	ng	993995	3	14.580	1356130	20.0
1-Decanamine, N...	19.333	25.6	ng	2306620	4	17.336	1801350	20.0
1-(Ethenesulfon...	21.272	5.2	ng	291826	5	21.595	1120110	20.0
Nonahexacontano...	22.447	3.1	ng	174425	5	21.595	1120110	20.0
Squalene	23.317	9.1	ng	548439	6	24.733	1210640	20.0
Heptadecane, 9-...	23.934	5.0	ng	300069	6	24.733	1210640	20.0