

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
 Data File : BG045069.D
 Acq On : 18 Apr 2020 16:23
 Operator : CG/JU
 Sample : L2271-13
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BG-10

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BG041520.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.118	3	5	14	rVB	58197	98056	2.06%	0.395%
2	3.195	14	18	24	rVB	42108	58565	1.23%	0.236%
3	5.591	419	426	435	rBV	809433	1341923	28.23%	5.408%
4	6.719	611	618	625	rVB	123484	209637	4.41%	0.845%
5	7.183	688	697	709	rBV	922763	1637397	34.44%	6.599%
6	8.023	833	840	847	rVB	196269	337411	7.10%	1.360%
7	8.346	887	895	902	rBV	713369	1270108	26.72%	5.118%
8	9.181	1027	1037	1046	rBV	580227	1091268	22.95%	4.398%
9	10.825	1310	1317	1325	rBV	281433	530320	11.16%	2.137%
10	13.281	1727	1735	1742	rBV	1896871	2979945	62.68%	12.009%
11	14.103	1868	1875	1881	rBV	215048	317665	6.68%	1.280%
12	14.656	1960	1969	1976	rBV2	542652	869963	18.30%	3.506%
13	16.142	2212	2222	2230	rBV	1813199	2826188	59.45%	11.389%
14	17.399	2430	2436	2444	rVB	756236	1157340	24.34%	4.664%
15	18.298	2582	2589	2596	rBV2	96796	183280	3.86%	0.739%
16	18.591	2634	2639	2643	rBV7	28879	48275	1.02%	0.195%
17	18.644	2643	2648	2652	rVB6	44499	73740	1.55%	0.297%
18	18.950	2694	2700	2703	rBV7	34836	57596	1.21%	0.232%
19	19.713	2823	2830	2835	rBV2	98628	128284	2.70%	0.517%
20	19.819	2841	2848	2854	rBV2	63974	135874	2.86%	0.548%
21	20.013	2874	2881	2887	rBV	3473346	4754053	100.00%	19.159%
22	20.154	2900	2905	2912	rBV8	82763	136098	2.86%	0.548%
23	20.483	2957	2961	2966	rVB7	39671	62839	1.32%	0.253%
24	20.647	2982	2989	2993	rBV4	150207	237874	5.00%	0.959%
25	20.683	2993	2995	3003	rVB9	41913	62829	1.32%	0.253%
26	20.753	3003	3007	3011	rBV2	181443	238640	5.02%	0.962%
27	20.800	3011	3015	3022	rVB10	52805	109763	2.31%	0.442%
28	21.317	3099	3103	3115	rBV	348379	514542	10.82%	2.074%
29	21.664	3155	3162	3171	rVB	717551	1220864	25.68%	4.920%
30	22.498	3299	3304	3320	rVB2	175563	412057	8.67%	1.661%
31	23.173	3414	3419	3426	rBV5	37024	72031	1.52%	0.290%
32	23.978	3552	3556	3560	rBV4	34142	57998	1.22%	0.234%
33	24.853	3695	3705	3713	rBV	400774	1144242	24.07%	4.611%
34	26.158	3921	3927	3940	rVB5	91736	296410	6.23%	1.195%

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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 >
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35	29.030	4408	4416	4418	rBV9	60144	141169	2.97%	0.569%
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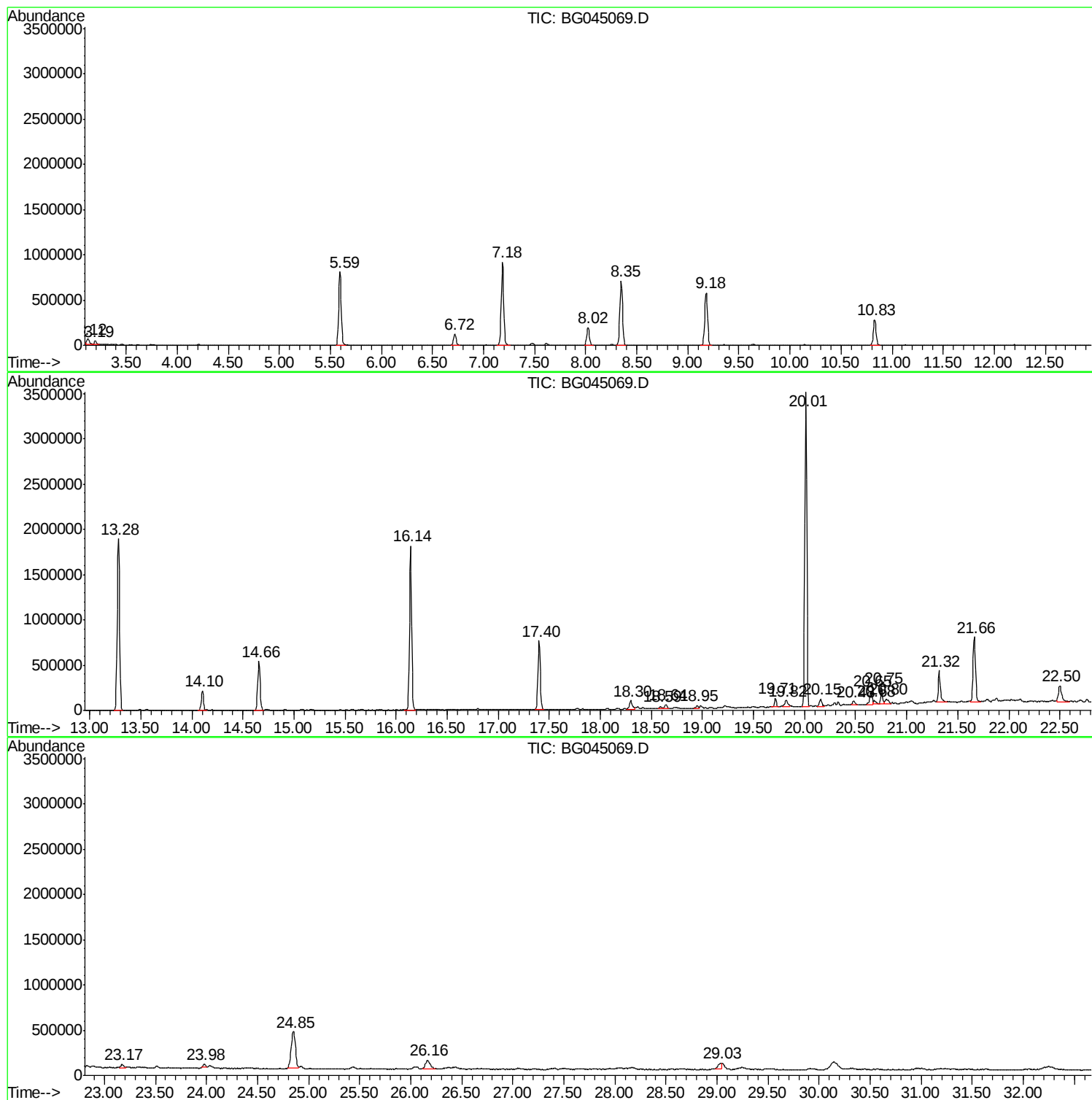
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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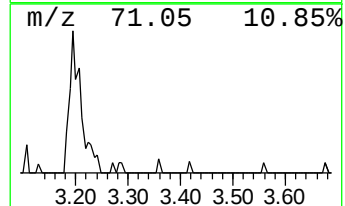
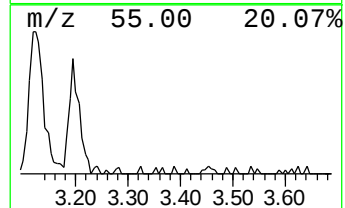
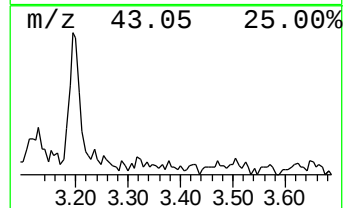
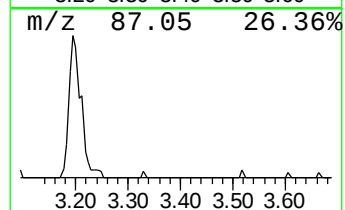
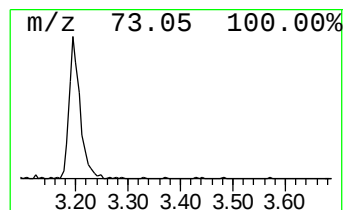
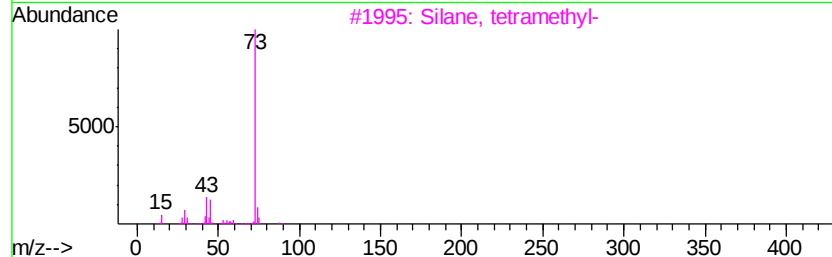
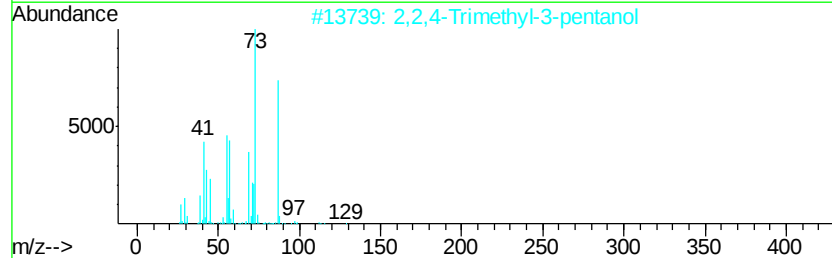
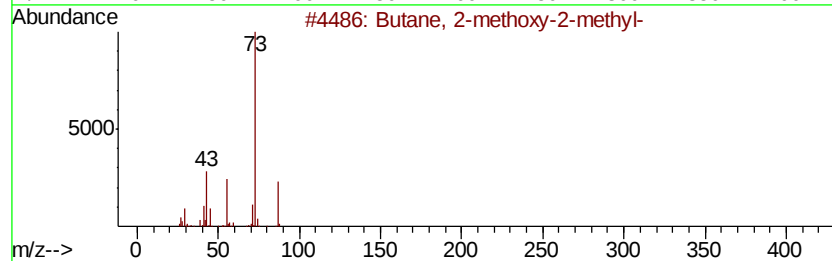
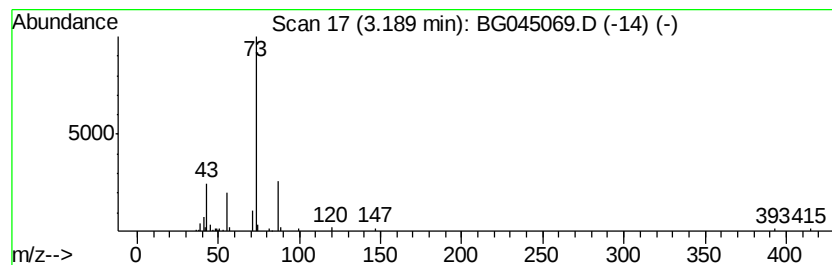
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	3.47 ng	58565	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4		Silane, trimethyl-2-penteny-, (E)-	142	C8H18Si	040795-28-6	9
5		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9



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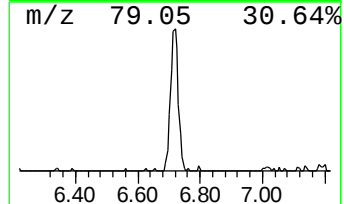
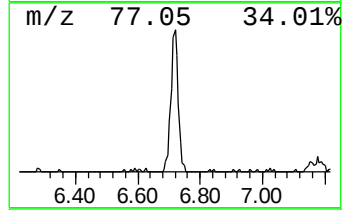
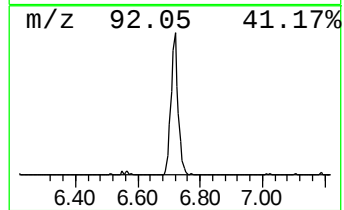
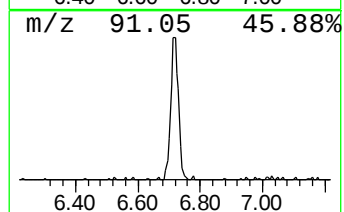
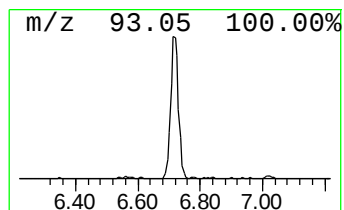
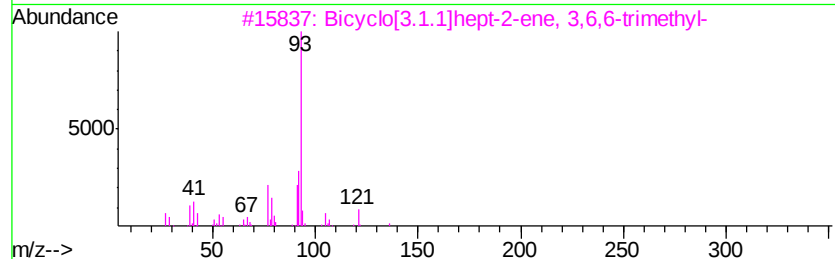
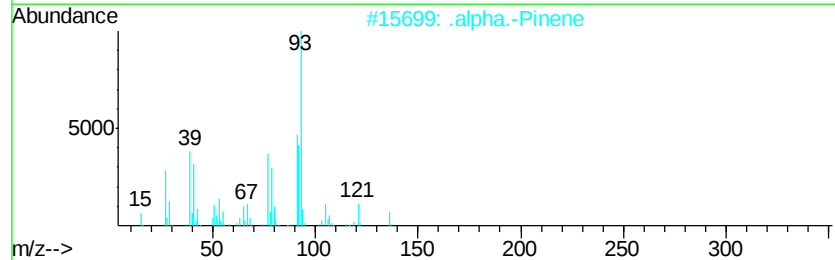
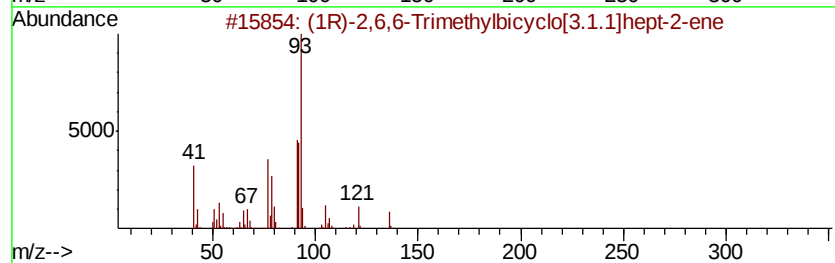
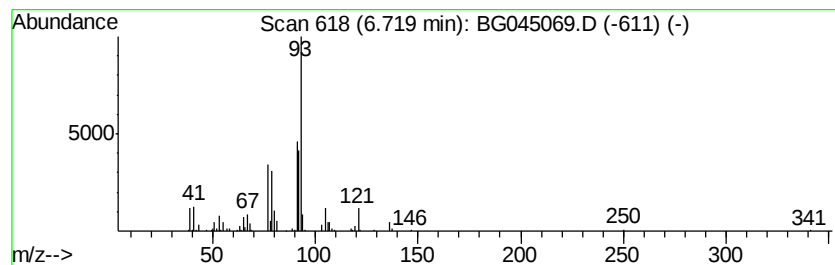
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	12.43 ng	209637	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	95
2		.alpha.-Pinene	136	C10H16	000080-56-8	95
3		Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91
4		trans-.beta.-Ocimene	136	C10H16	003779-61-1	86
5		(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	83



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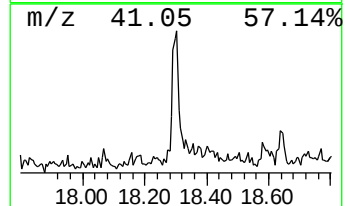
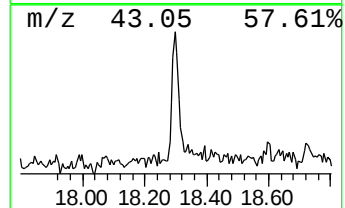
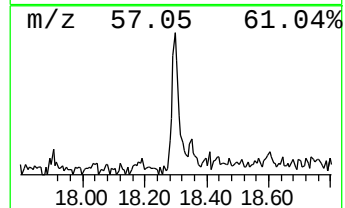
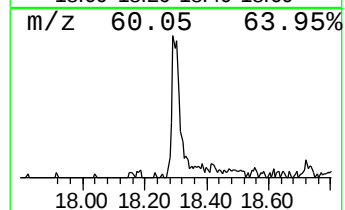
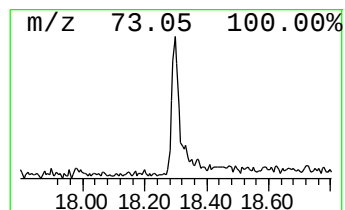
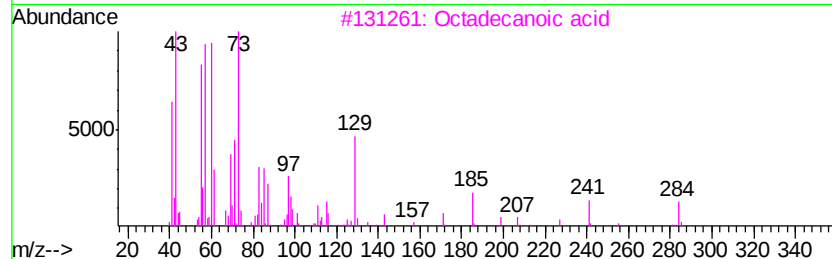
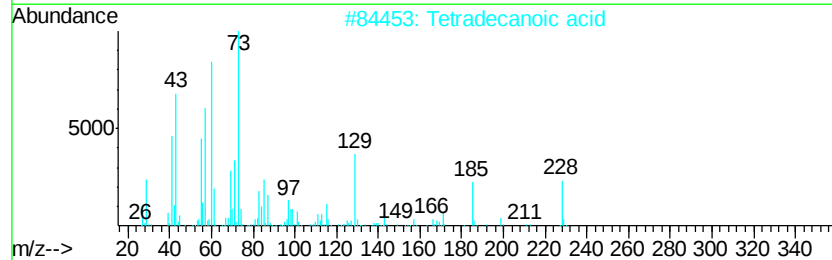
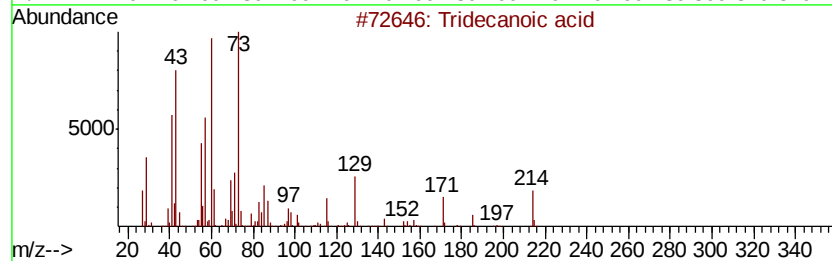
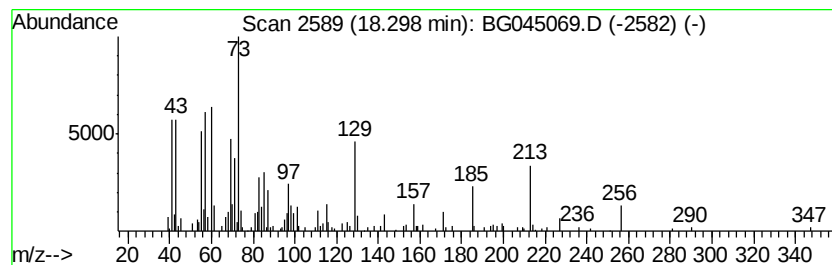
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.17 ng	183280	Phenanthrene-d10	17.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	89
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		Octadecanoic acid	284	C18H36O2	000057-11-4	64
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
5		Undecanoic acid	186	C11H22O2	000112-37-8	47



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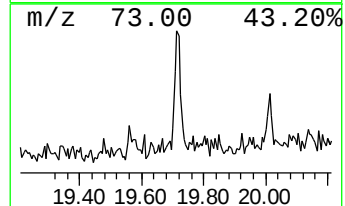
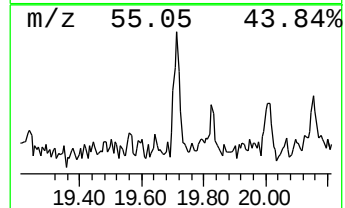
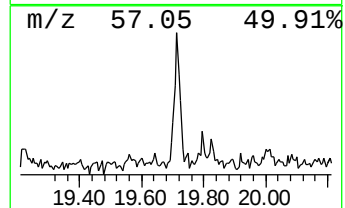
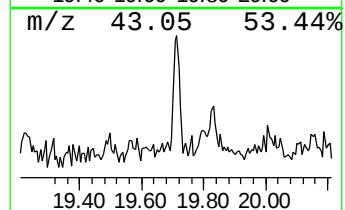
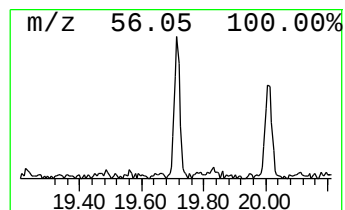
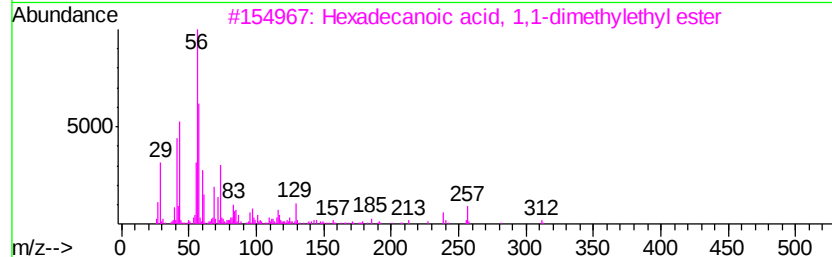
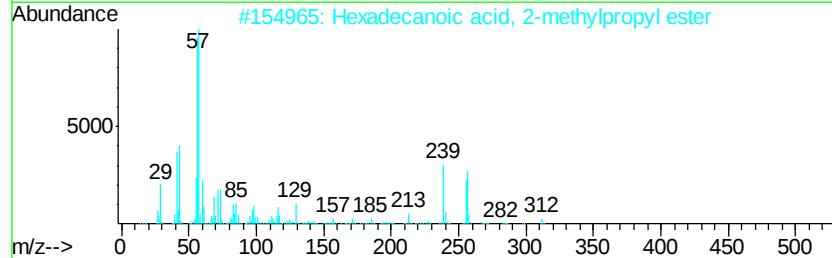
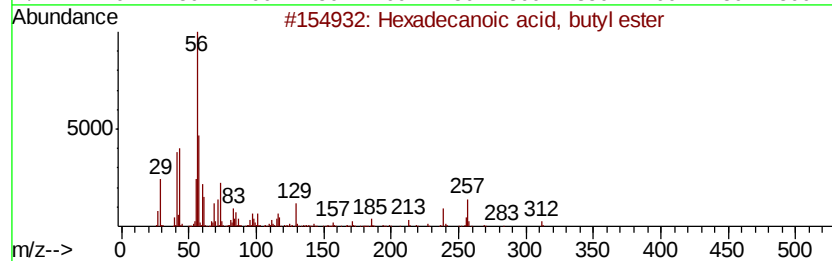
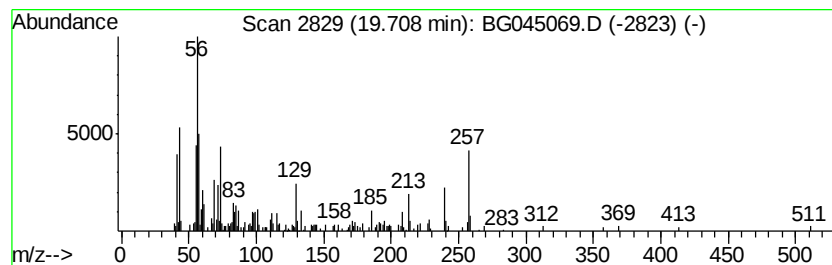
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.71	2.10 ng	128284	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	55
2		Hexadecanoic acid, 2-methylpropyl ester	312	C20H40O2	000110-34-9	53
3		Hexadecanoic acid, 1,1-dimethylethyl ester	312	C20H40O2	031158-91-5	46
4		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	22
5		Cyclopentanone, 2,2,5,5-tetramethyl-	140	C9H16O	004541-35-9	22



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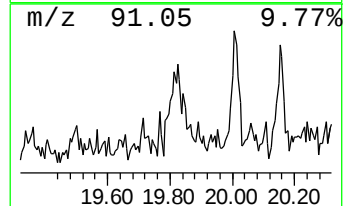
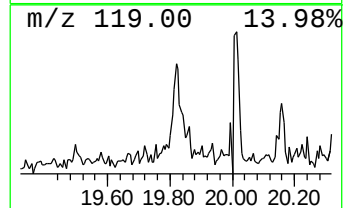
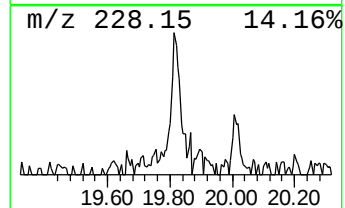
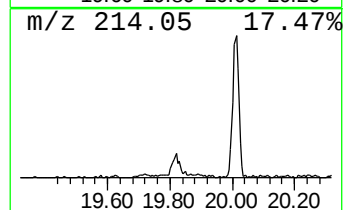
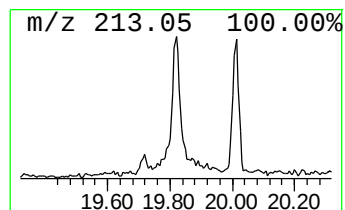
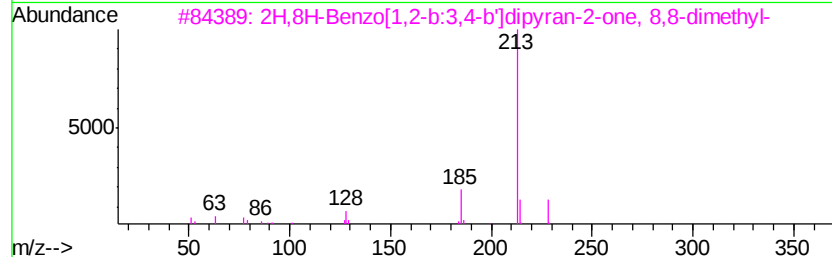
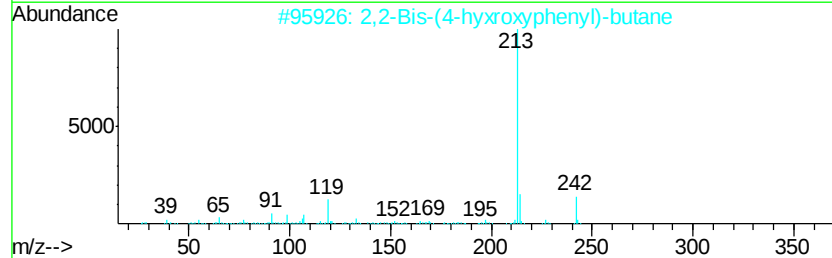
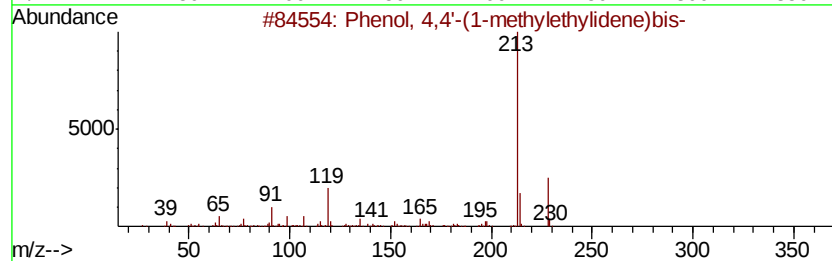
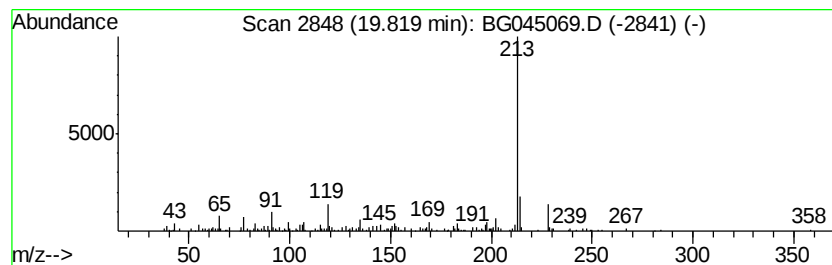
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Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.82	2.23 ng	135874	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	93
2		2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	72
3		2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	64
4		Indole,6-methyl-2-(2-thienyl)-	213	C13H11NS	296245-70-0	64
5		2,2'-Bis(p-acetoxyphenyl)propane	312	C19H20O4	010192-62-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045069.D
Acq On : 18 Apr 2020 16:23
Operator : CG/JU
Sample : L2271-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BG-10

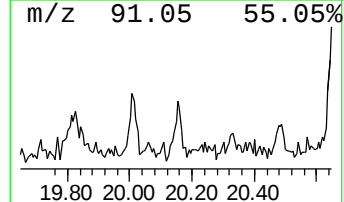
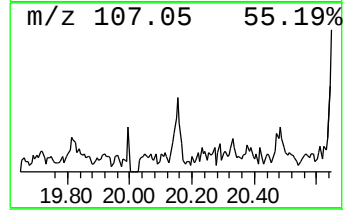
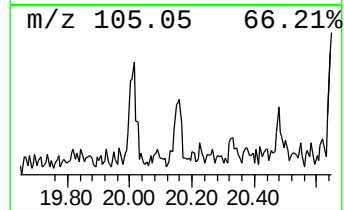
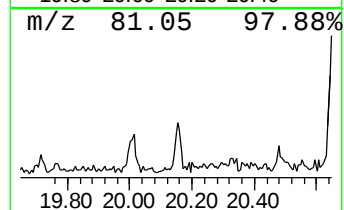
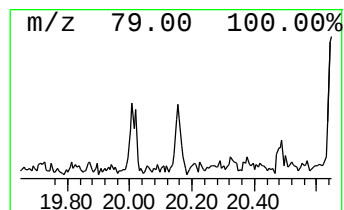
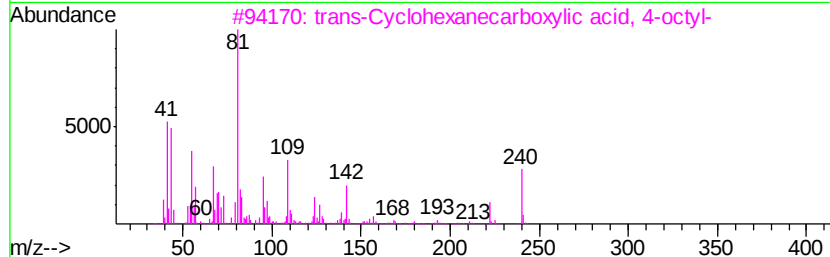
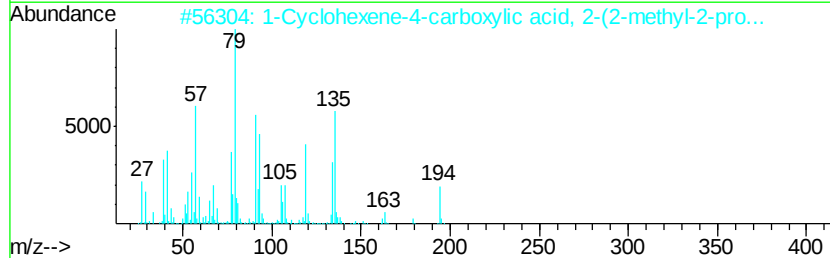
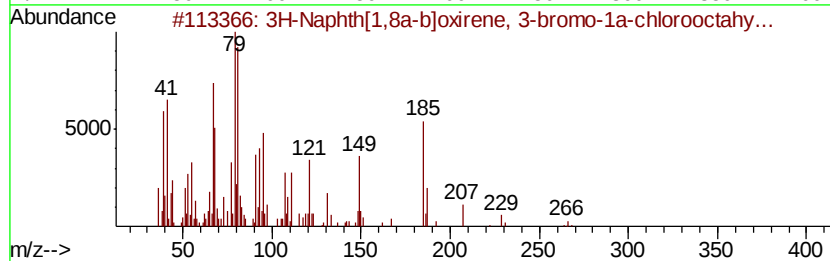
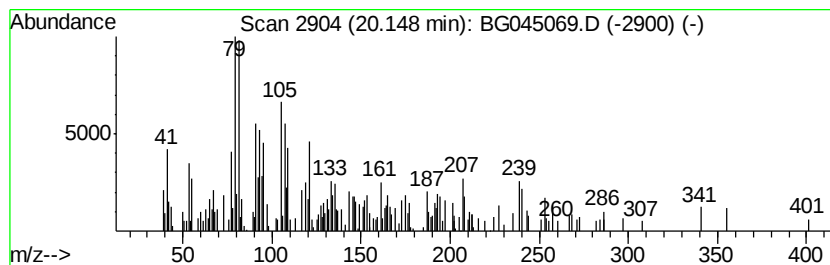
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown20.15 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.15	2.23 ng	136098	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3H-Naphth[1,8a-b]oxirene, 3-brom...	264	C10H14BrClO	1000141-72-2	32
2		1-Cyclohexene-4-carboxylic acid,...	194	C12H18O2	1000154-18-9	30
3		trans-Cyclohexanecarboxylic acid...	240	C15H28O2	038289-32-6	25
4		1-Cyclohexene-4-carboxylic acid,...	194	C12H18O2	1000154-19-0	25
5		Tricyclo[7.4.0.0(3,8)]trideca-5,...	240	C17H20O	1000157-14-9	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045069.D
Acq On : 18 Apr 2020 16:23
Operator : CG/JU
Sample : L2271-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

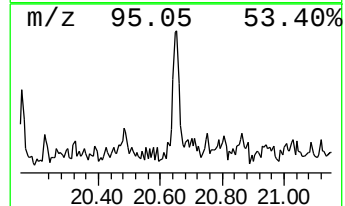
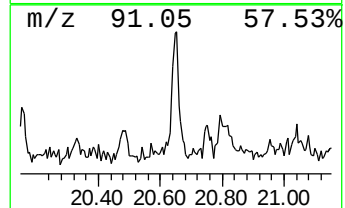
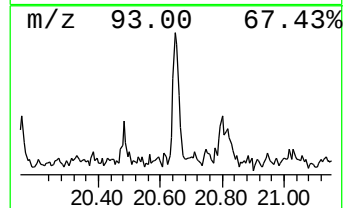
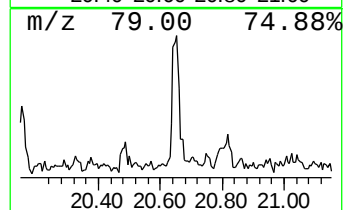
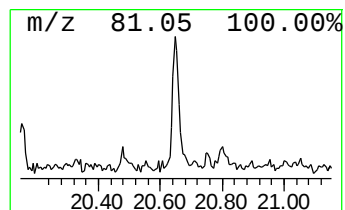
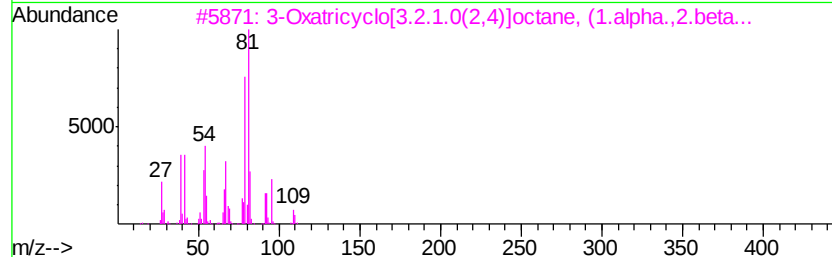
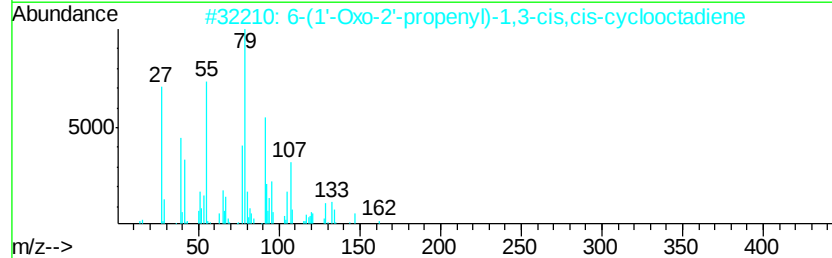
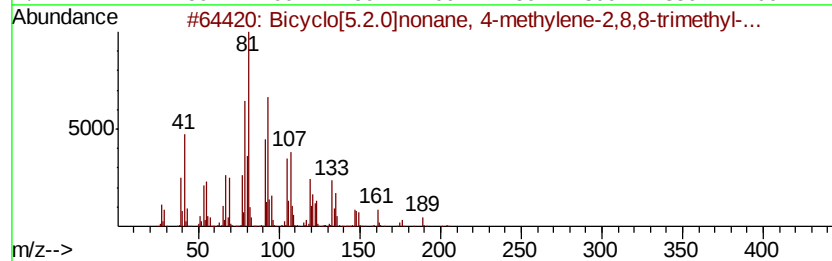
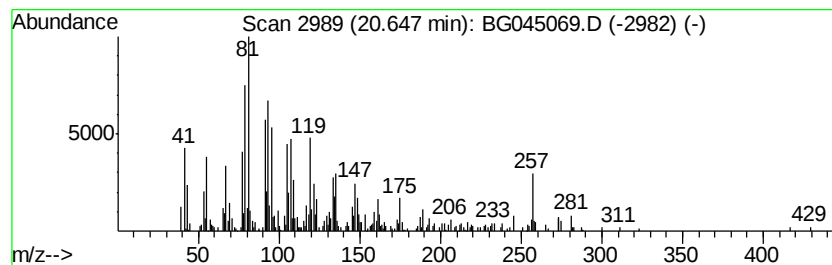
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bicyclo[5.2.0]nonane, 4-met... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.65	3.90 ng	237874	Chrysene-d12	21.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Bicyclo[5.2.0]nonane, 4-methylen...	204	C15H24	1000159-38-2 52
2	6-(1'-Oxo-2'-propenyl)-1,3-cis,c...	162	C11H14O	138146-05-1 41
3	3-Oxatricyclo[3.2.1.0(2,4)]octan...	110	C7H10O	003146-39-2 38
4	3-Tetradecen-5-yne, (E)-	192	C14H24	074744-44-8 35
5	10,12-Tricosadiynoic acid, methy...	360	C24H40O2	1000333-59-4 18



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045069.D
Acq On : 18 Apr 2020 16:23
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Misc :
ALS Vial : 42 Sample Multiplier: 1

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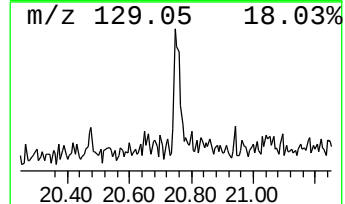
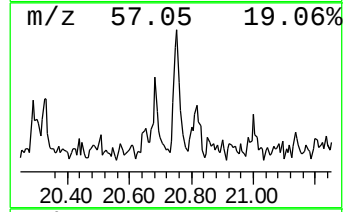
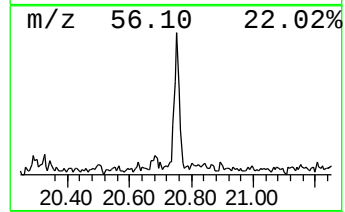
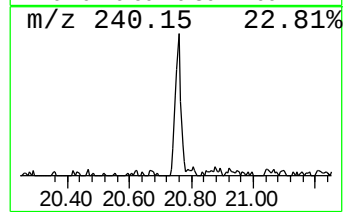
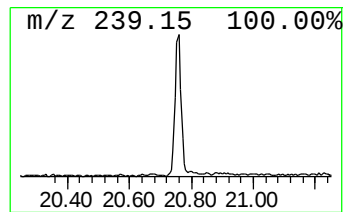
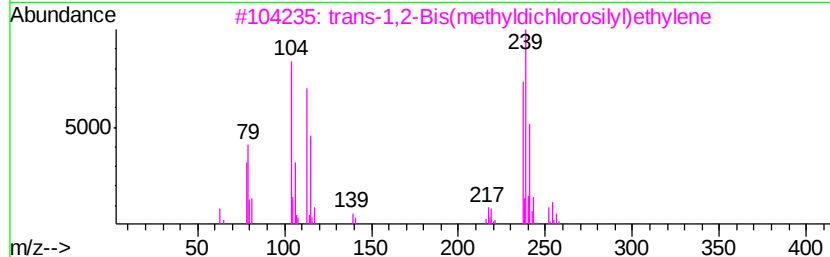
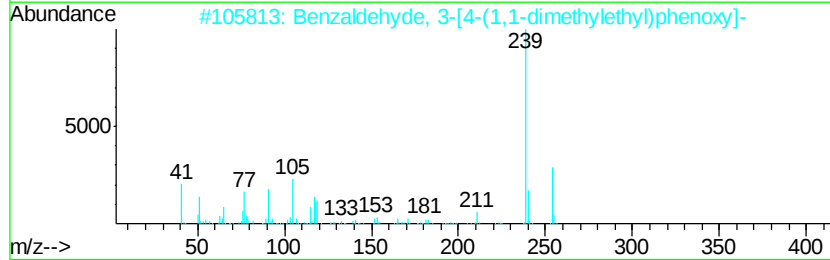
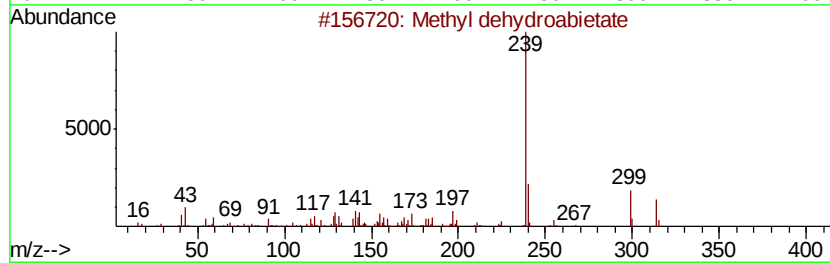
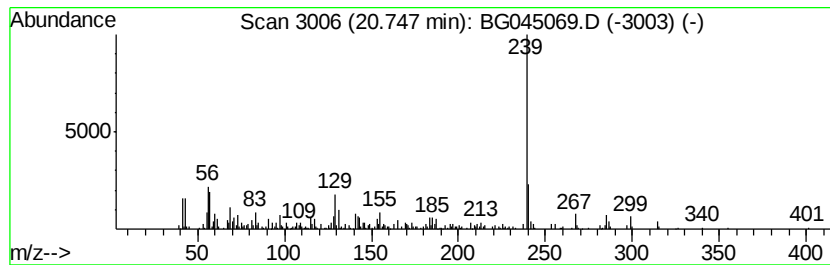
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Methyl dehydroabietate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.75	3.91 ng	238640	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl dehydroabietate	314	C21H30O2	001235-74-1	86
2		Benzaldehyde, 3-[4-(1,1-dimethyl...	254	C17H18O2	069770-23-6	50
3		trans-1,2-Bis(methyldichlorosilyl...	252	C4H8Cl4Si2	065899-10-7	50
4		1-[4-(4-Chlorophenyl)thioxomethyl]...	239	C12H14ClNS	003335-29-3	50
5		Dehydroabietic acid, trimethylsi...	372	C23H36O2Si	021414-49-3	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045069.D
Acq On : 18 Apr 2020 16:23
Operator : CG/JU
Sample : L2271-13
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BG-10

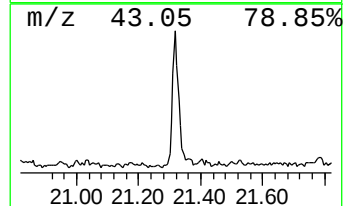
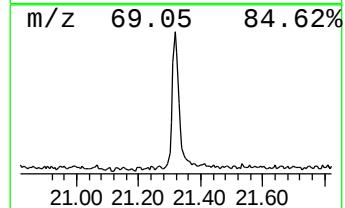
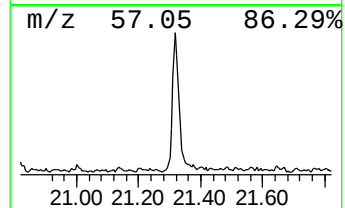
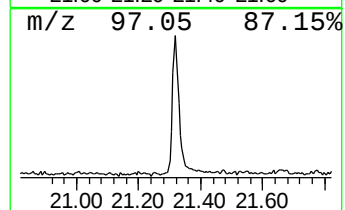
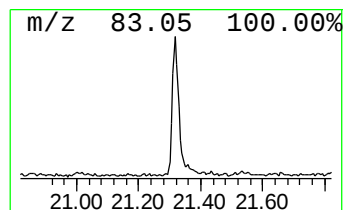
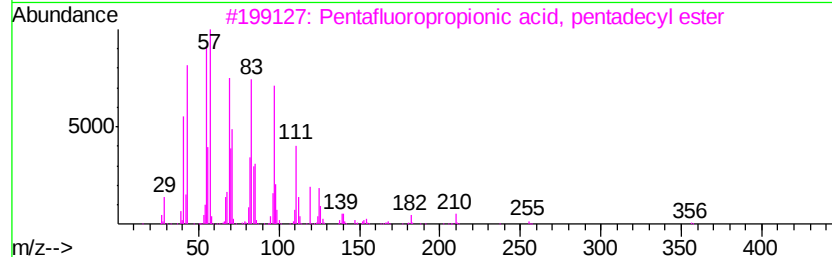
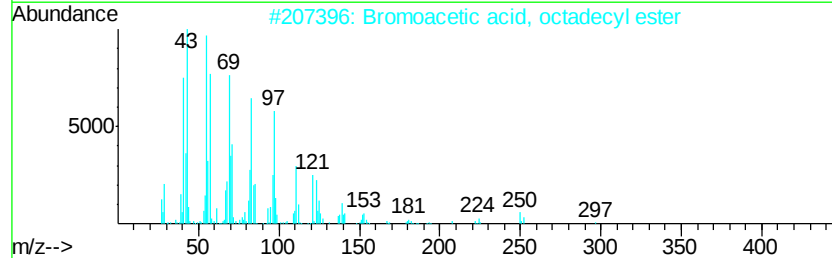
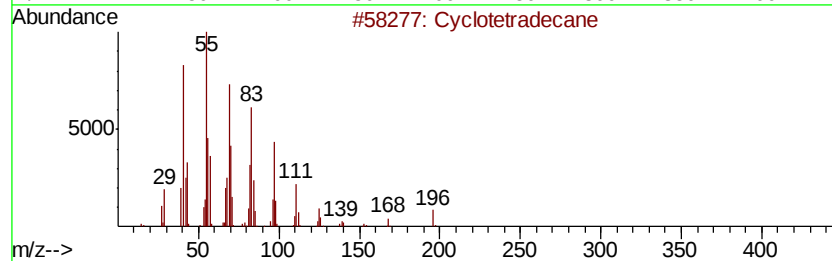
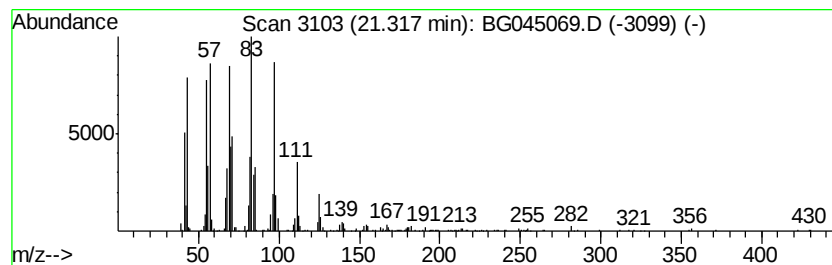
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclotetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	8.43 ng	514542	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotetradecane	196	C14H28	000295-17-0	93
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5		Isoheptadecanol	256	C17H36O	057289-07-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045069.D
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Sample : L2271-13
Misc :
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Instrument :
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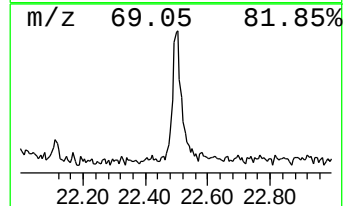
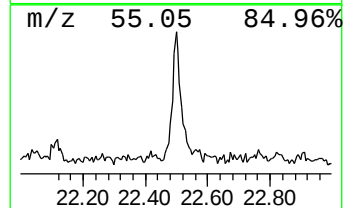
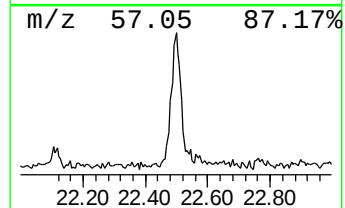
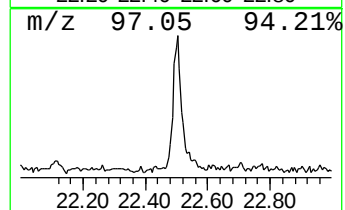
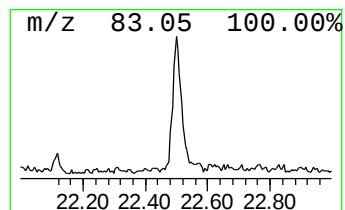
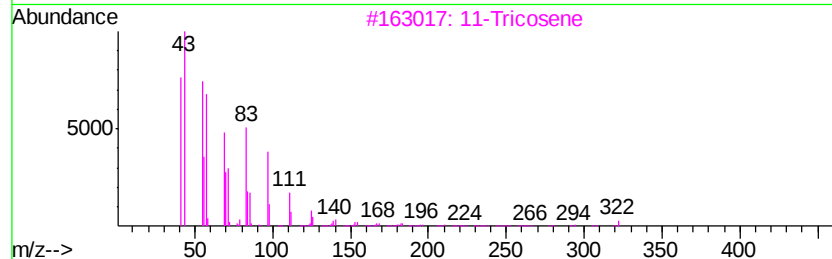
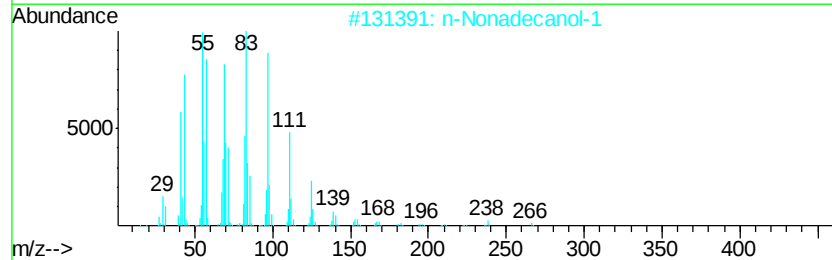
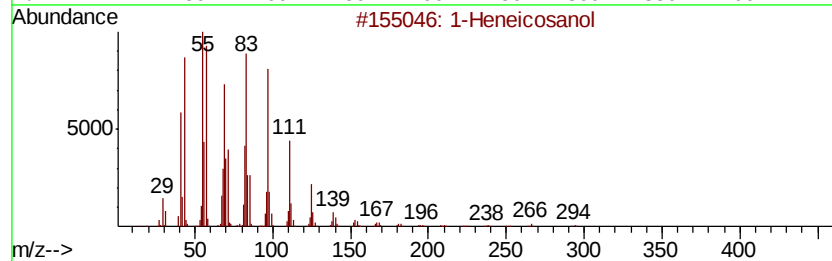
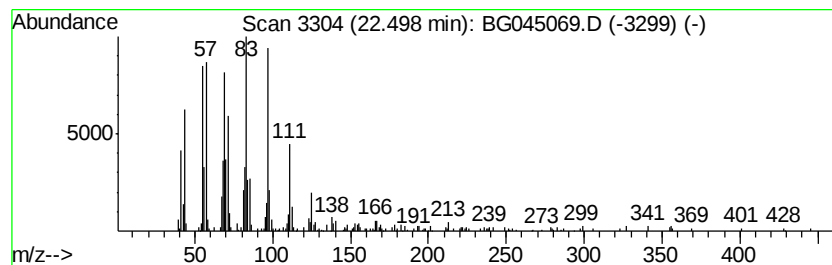
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.50	6.75 ng	412057	Chrysene-d12	21.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	91
2	n-Nonadecanol-1		284	C19H40O	001454-84-8	91
3	11-Tricosene		322	C23H46	052078-56-5	91
4	Cyclohexadecane		224	C16H32	000295-65-8	90
5	Behenic alcohol		326	C22H46O	000661-19-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045069.D
Acq On : 18 Apr 2020 16:23
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ClientSampleId :
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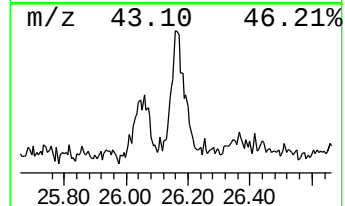
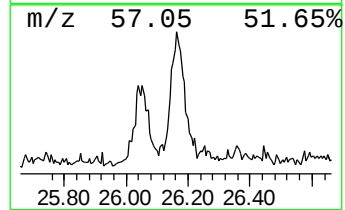
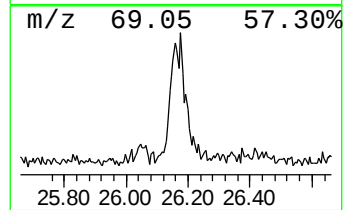
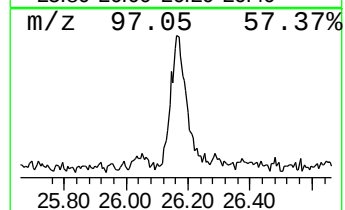
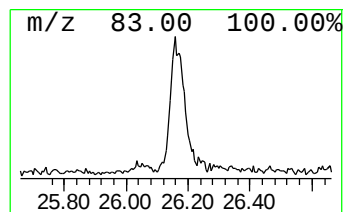
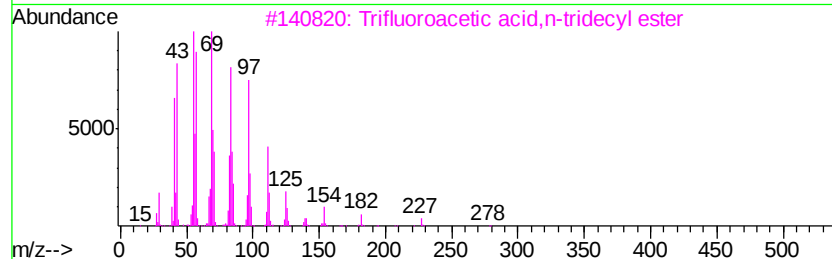
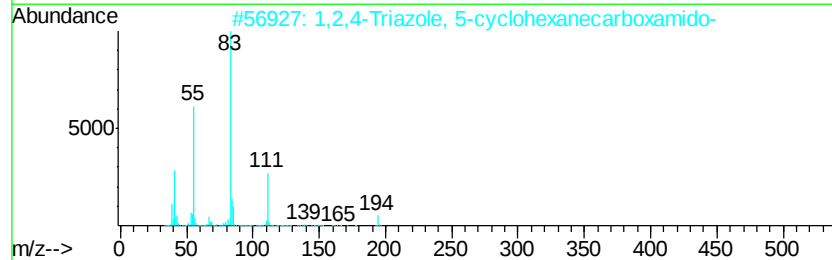
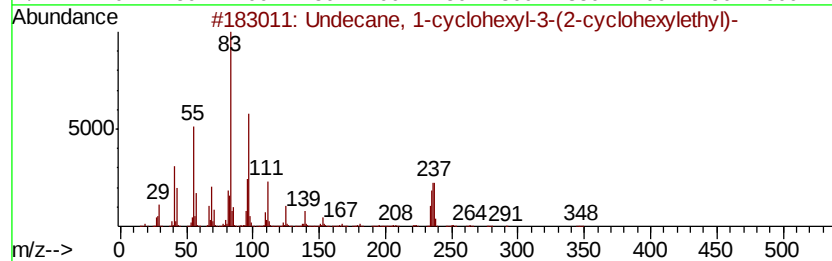
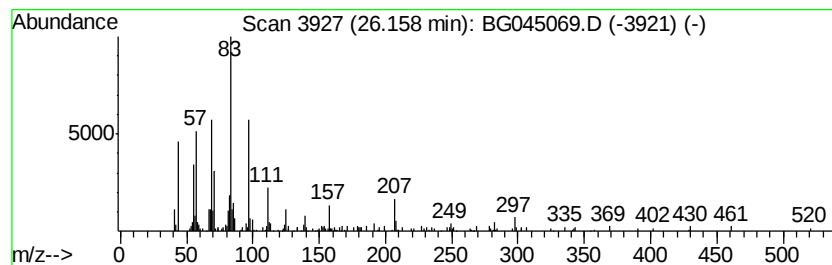
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Undecane, 1-cyclohexyl-3-(2... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.16	5.18 ng	296410	Perylene-d12	24.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 1-cyclohexyl-3-(2-cycl...	348	C25H48	007225-69-6	72
2		1,2,4-Triazole, 5-cyclohexanecar...	194	C9H14N4O	021051-17-2	47
3		Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	47
4		1-Tridecyl-4-ol	196	C13H24O	074646-37-0	47
5		3-Decen-5-one	154	C10H18O	032064-73-6	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045069.D
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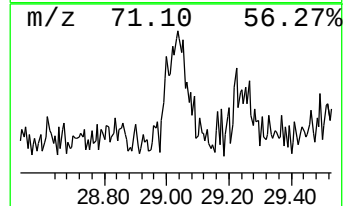
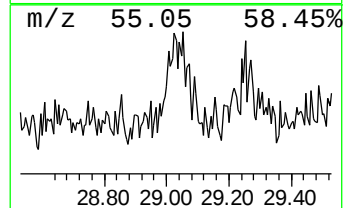
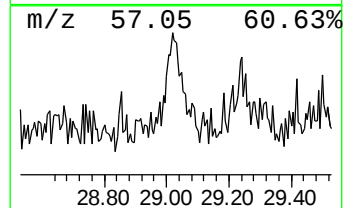
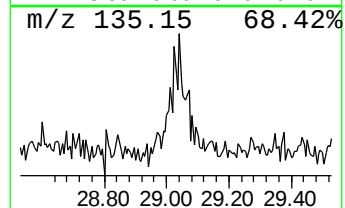
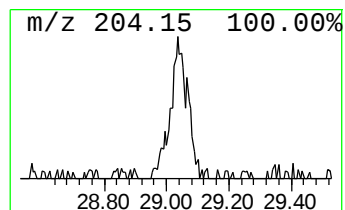
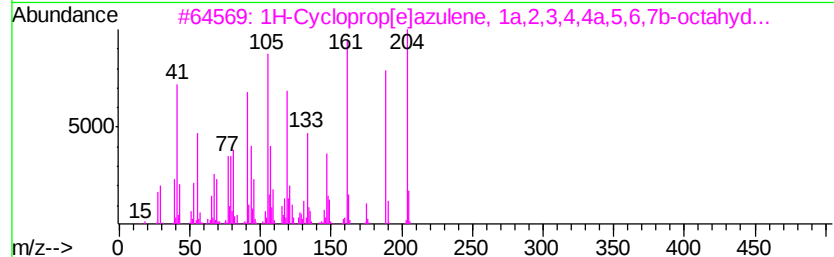
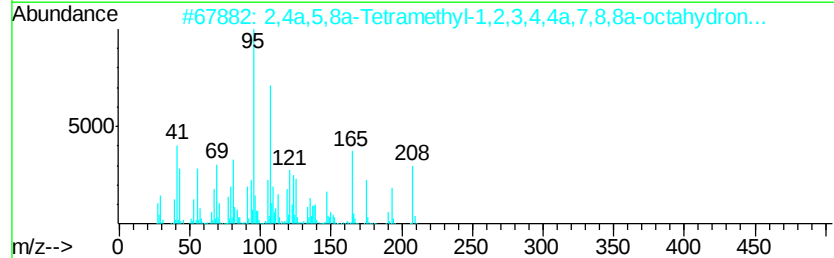
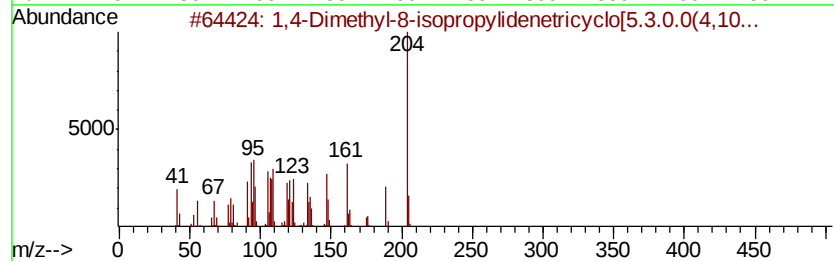
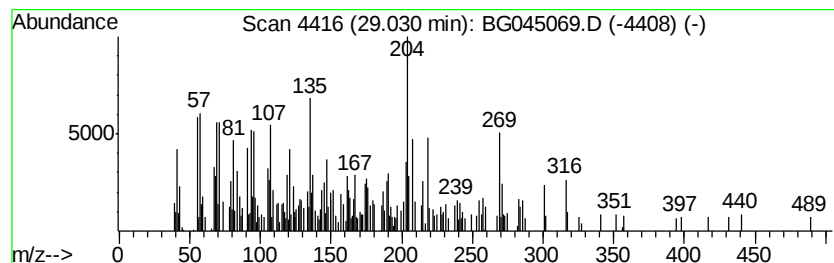
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown29.03 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.03	2.47 ng	141169	Perylene-d12	24.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	35
2		2,4a,5,8a-Tetramethyl-1,2,3,4,4a...	208	C14H24O	020558-22-9	30
3		1H-Cycloprop[elazulene, 1a,2,3,4...	204	C15H24	000489-40-7	30
4		Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	27
5		1,4-Methanoazulen-9-ol, decahydr...	222	C15H26O	000465-24-7	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG041720\
 Data File : BG045069.D
 Acq On : 18 Apr 2020 16:23
 Operator : CG/JU
 Sample : L2271-13
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BG-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041520.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
Butane, 2-methoxy...	3.19	3.5	ng	58565	1	8.02	337411	20.0
(1R)-2,6,6-Trimet...	6.72	12.4	ng	209637	1	8.02	337411	20.0
Tridecanoic acid	18.30	3.2	ng	183280	4	17.40	1157340	20.0
Hexadecanoic acid...	19.71	2.1	ng	128284	5	21.66	1220860	20.0
Phenol, 4,4'-(1-m...	19.82	2.2	ng	135874	5	21.66	1220860	20.0
unknown20.15	20.15	2.2	ng	136098	5	21.66	1220860	20.0
Bicyclo[5.2.0]non...	20.65	3.9	ng	237874	5	21.66	1220860	20.0
Methyl dehydroabi...	20.75	3.9	ng	238640	5	21.66	1220860	20.0
Cyclotetradecane	21.32	8.4	ng	514542	5	21.66	1220860	20.0
1-Heneicosanol	22.50	6.8	ng	412057	5	21.66	1220860	20.0
Undecane, 1-cyclo...	26.16	5.2	ng	296410	6	24.85	1144240	20.0
unknown29.03	29.03	2.5	ng	141169	6	24.85	1144240	20.0