

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
 Data File : BG045076.D
 Acq On : 18 Apr 2020 21:00
 Operator : CG/JU
 Sample : L2271-08
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DUP-2020-04-13

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	3.123	3	6	14	rVB2	58046	92656	1.46%	0.309%
2	3.194	14	18	26	rVB	45849	71282	1.12%	0.238%
3	5.591	419	426	436	rBV	1048189	1736300	27.38%	5.798%
4	6.719	611	618	624	rVB	213824	361189	5.69%	1.206%
5	7.183	687	697	708	rBV	1230444	2177880	34.34%	7.272%
6	7.471	741	746	753	rVB3	40857	72043	1.14%	0.241%
7	8.023	833	840	847	rBV	209997	367511	5.79%	1.227%
8	8.346	885	895	908	rBV	981832	1735112	27.36%	5.794%
9	9.174	1028	1036	1046	rBV	805520	1492719	23.53%	4.985%
10	10.831	1309	1318	1325	rBV	298548	559508	8.82%	1.868%
11	13.280	1726	1735	1742	rBV	2575299	4100412	64.65%	13.692%
12	14.103	1869	1875	1881	rBV	271198	402686	6.35%	1.345%
13	14.655	1962	1969	1978	rVB	586065	919471	14.50%	3.070%
14	16.141	2213	2222	2234	rBV	2389320	3783421	59.65%	12.634%
15	17.398	2427	2436	2443	rBV	765201	1194430	18.83%	3.988%
16	18.297	2583	2589	2594	rBV2	68543	111103	1.75%	0.371%
17	19.554	2799	2803	2807	rBV5	45372	68361	1.08%	0.228%
18	19.819	2841	2848	2855	rBV	59865	121771	1.92%	0.407%
19	20.012	2875	2881	2887	rBV	4535279	6342574	100.00%	21.179%
20	20.476	2956	2960	2967	rBV9	51316	83271	1.31%	0.278%
21	20.653	2986	2990	2992	rBV3	72528	88136	1.39%	0.294%
22	20.688	2992	2996	3002	rVB4	74735	132378	2.09%	0.442%
23	20.753	3003	3007	3012	rVB	132236	174215	2.75%	0.582%
24	20.823	3015	3019	3023	rVB6	47851	65570	1.03%	0.219%
25	21.317	3099	3103	3113	rVB	297160	455919	7.19%	1.522%
26	21.663	3155	3162	3170	rVB	753732	1245250	19.63%	4.158%
27	22.497	3298	3304	3316	rVB2	183863	413966	6.53%	1.382%
28	22.703	3336	3339	3346	rVB6	39859	76181	1.20%	0.254%
29	24.847	3695	3704	3714	rBV	431218	1182134	18.64%	3.947%
30	26.163	3920	3928	3938	rBV8	64543	214121	3.38%	0.715%
31	30.146	4598	4606	4607	rBV8	45513	105512	1.66%	0.352%

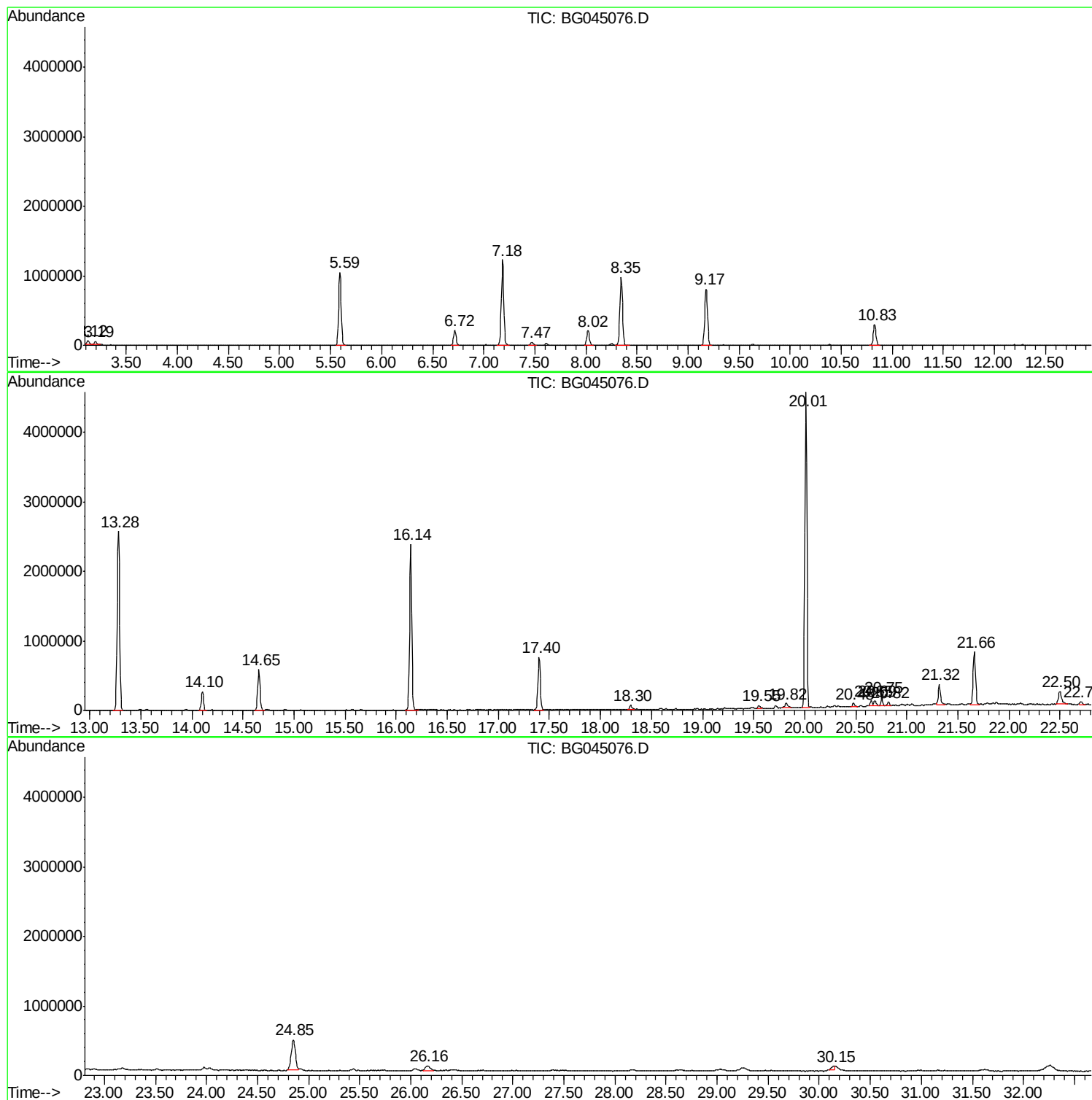
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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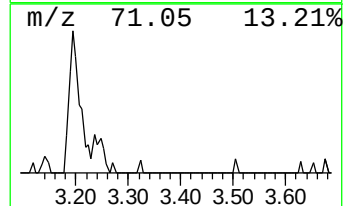
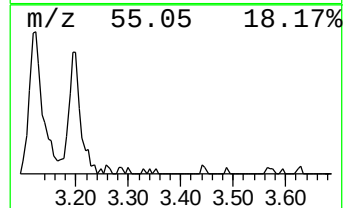
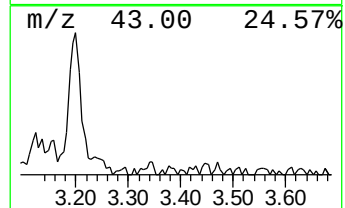
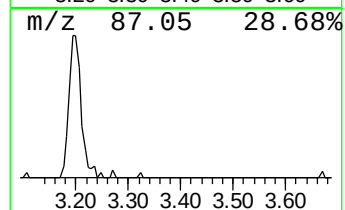
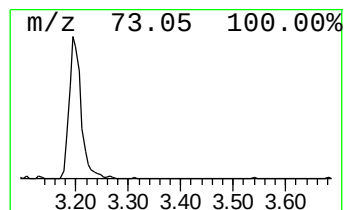
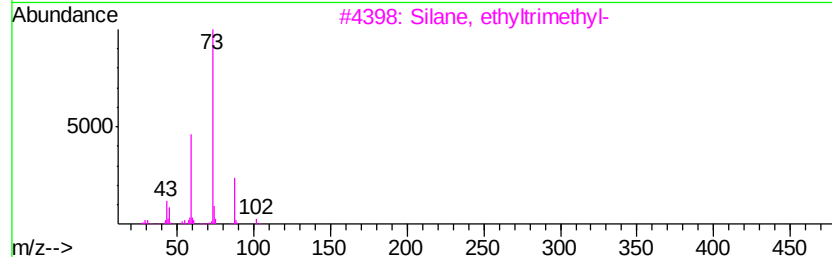
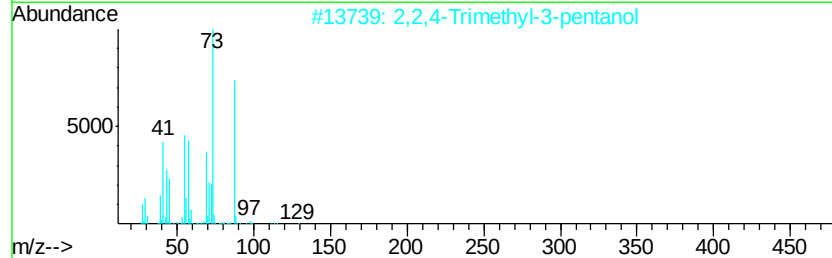
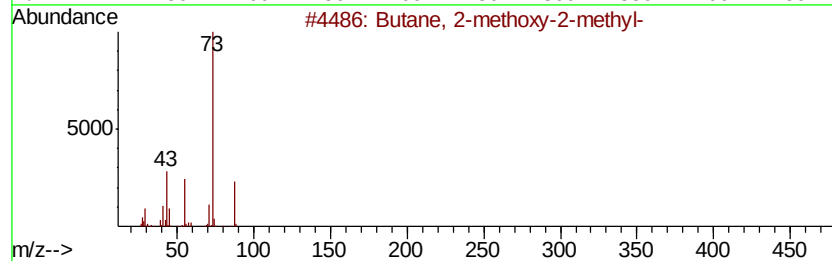
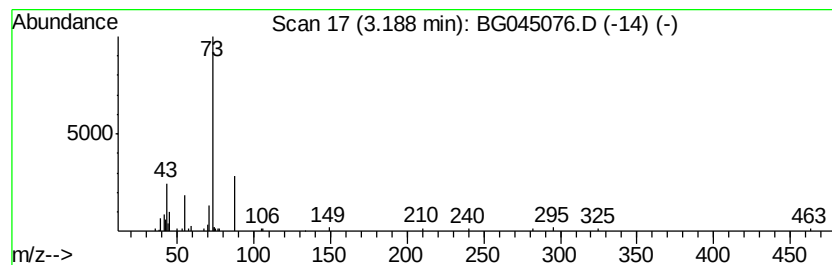
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	3.88 ng	71282	1,4-Dichlorobenzene-d4	8.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	45
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5			1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9



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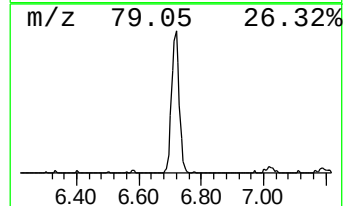
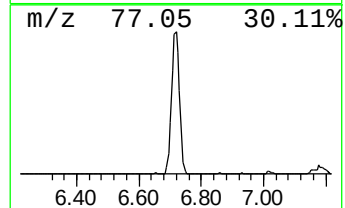
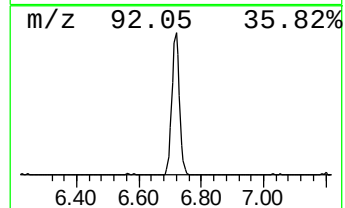
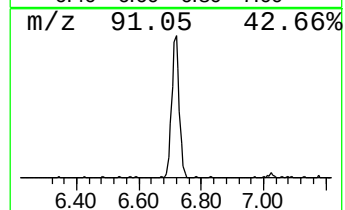
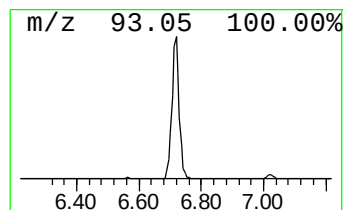
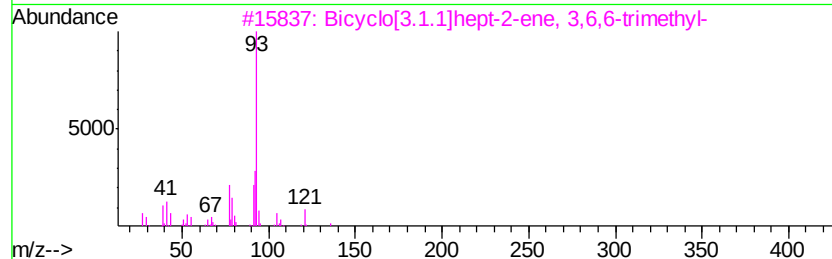
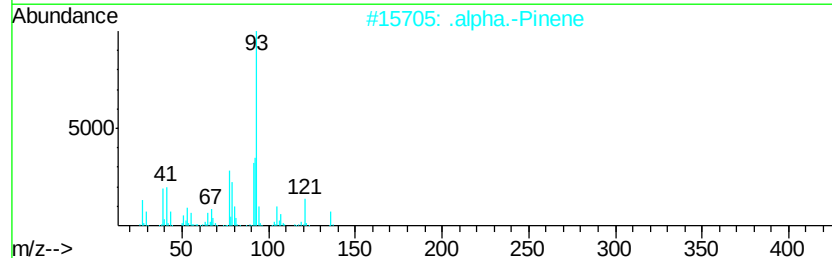
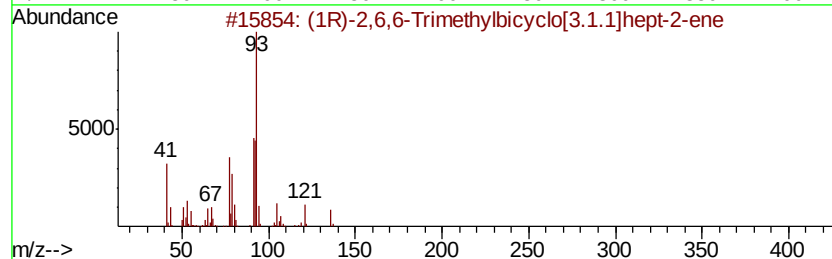
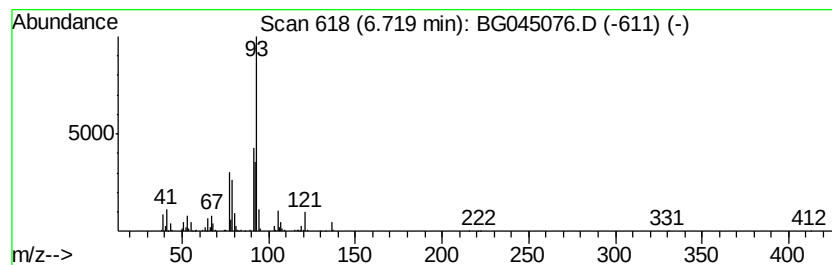
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	19.66 ng	361189	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	94
3		Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91
4		(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	91
5		Tricyclo[2.2.1.0(2,6)]heptane, 1,4-dichloro-	136	C10H16	000508-32-7	87



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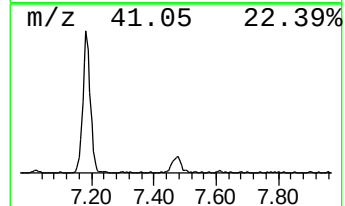
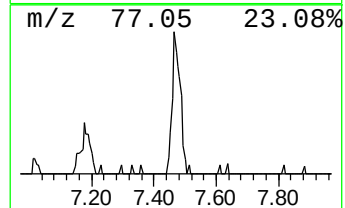
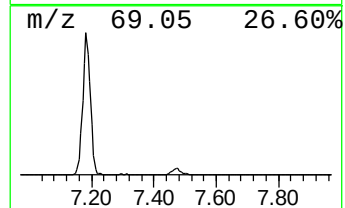
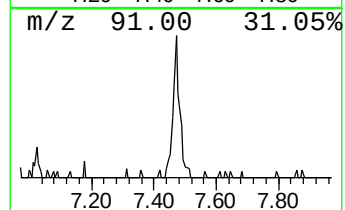
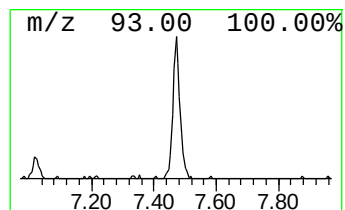
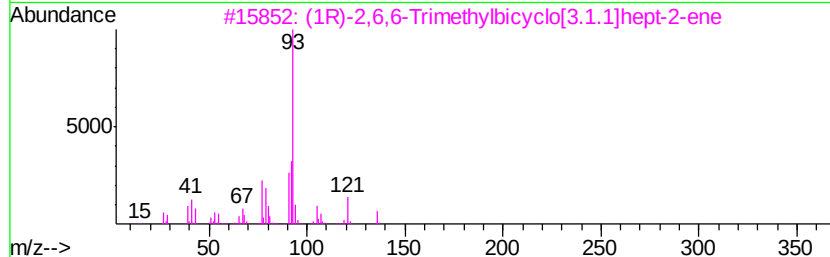
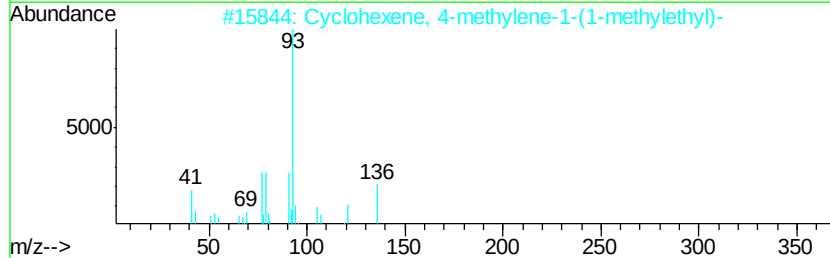
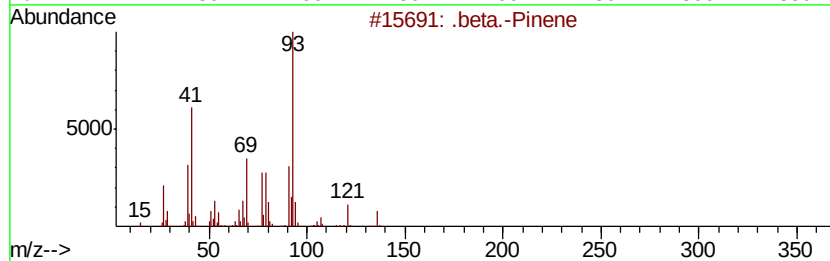
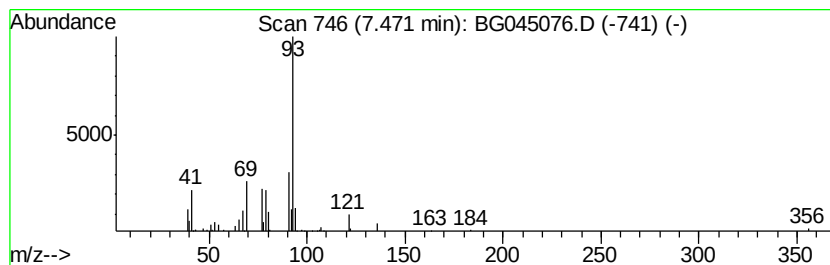
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 .beta.-Pinene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	3.92 ng	72043	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Pinene	136	C10H16	000127-91-3	94
2		Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	90
3		(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	87
4		Bicyclo[3.1.0]hex-2-ene, 4-methy...	136	C10H16	028634-89-1	87
5		Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	86



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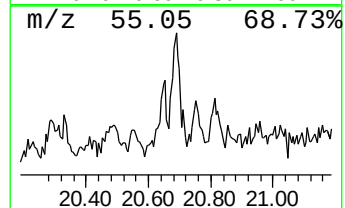
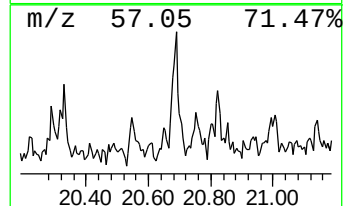
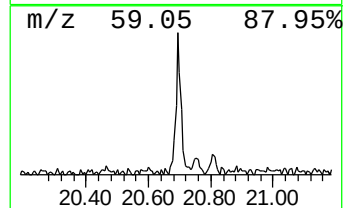
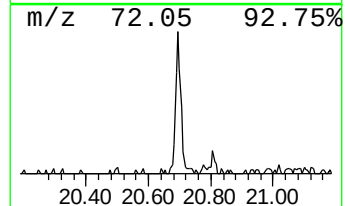
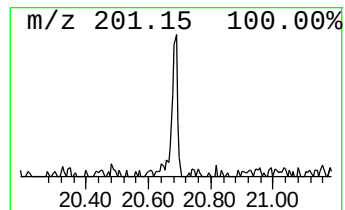
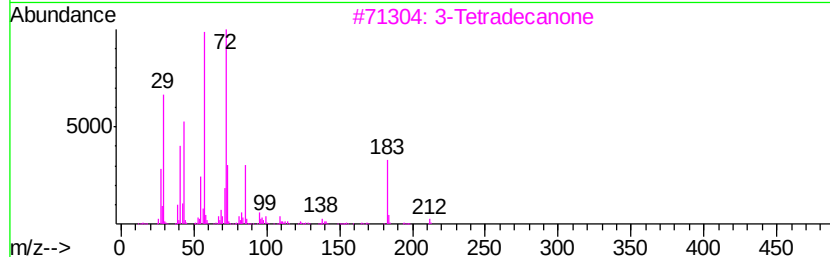
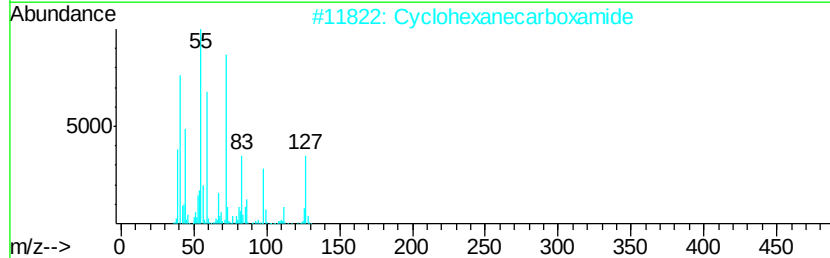
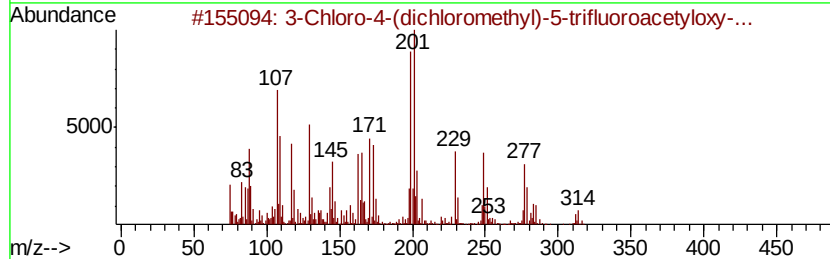
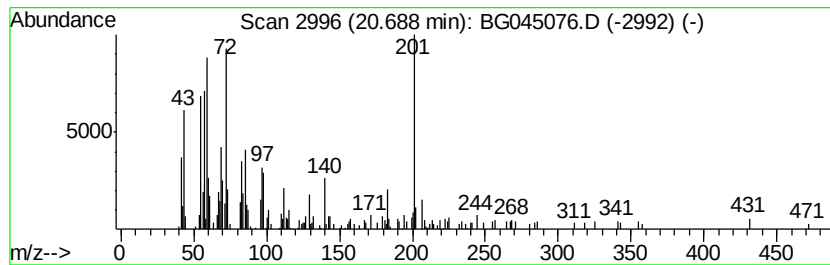
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Peak Number 6 unknown20.69 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.69	2.13 ng	132378	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-4-(dichloromethyl)-5-tr...	312	C7H2Cl3F3O4	1192024-37-5	22
2		Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	22
3		3-Tetradecanone	212	C14H28O	000629-23-2	20
4		Octadecanoic acid, 2-(octadecylo...	581	C38H76O3	028843-25-6	11
5		Thieno(2,3-b)quinoline-9-oxide	201	C11H7NOS	094734-32-4	11



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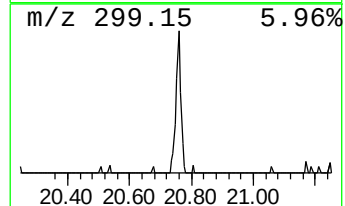
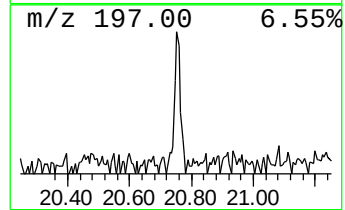
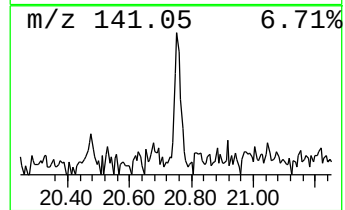
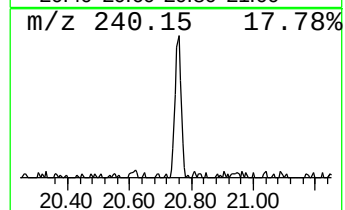
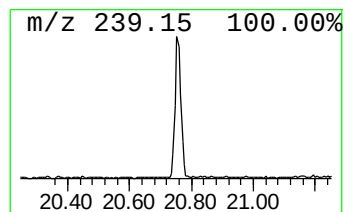
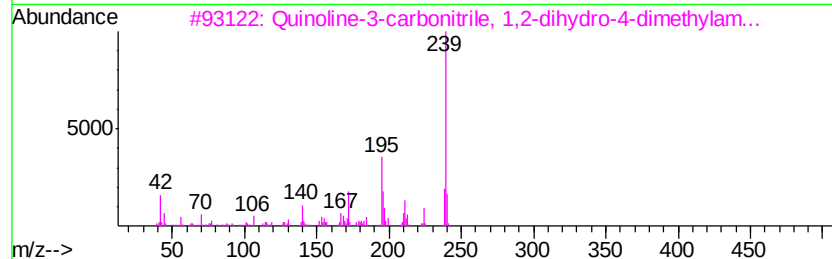
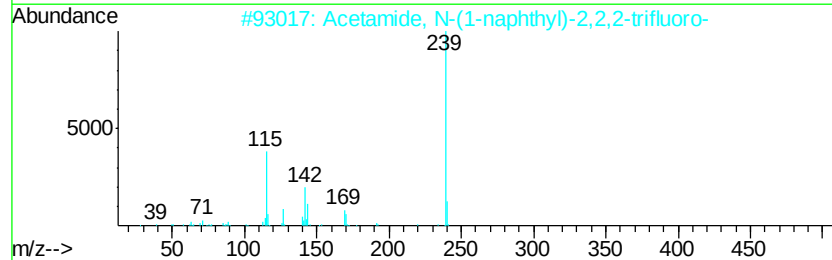
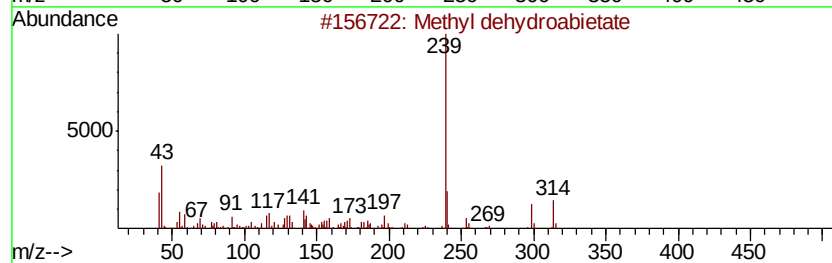
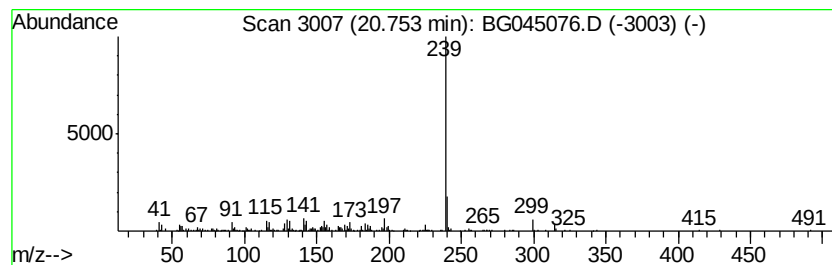
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 Peak Number 7 Methyl dehydroabietate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.75	2.80 ng	174215	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl dehydroabietate	314	C21H30O2	001235-74-1	91
2		Acetamide, N-(1-naphthyl)-2,2,2-...	239	C12H8F3NO	1000307-31-6	64
3		Quinoline-3-carbonitrile, 1,2-di...	239	C14H13N3O	209617-30-1	64
4		Cobalt, (.eta.5-2,4-cyclopentadi...	239	C14H12Co	088242-61-9	59
5		3,4-Dimethoxymandelic acid, di-TMS	356	C16H28O5Si2	1000072-02-7	56



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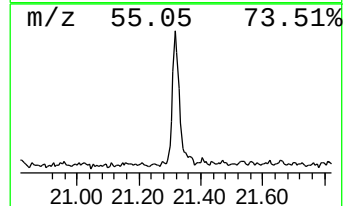
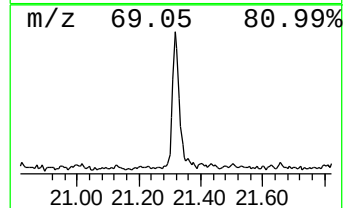
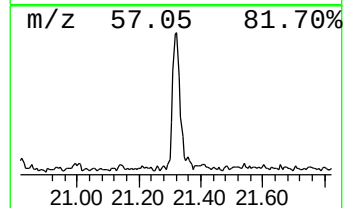
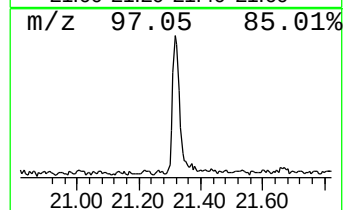
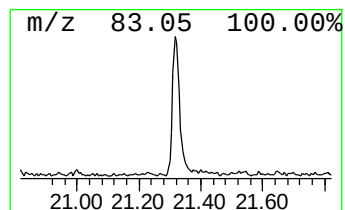
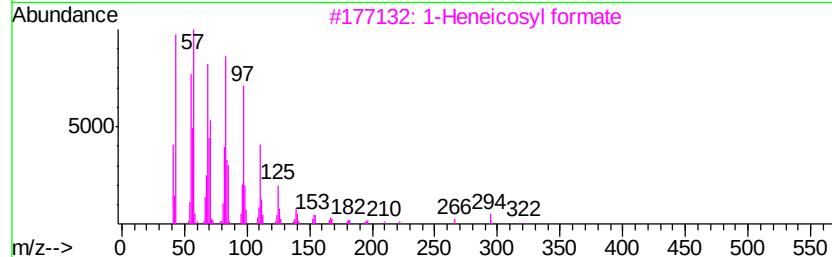
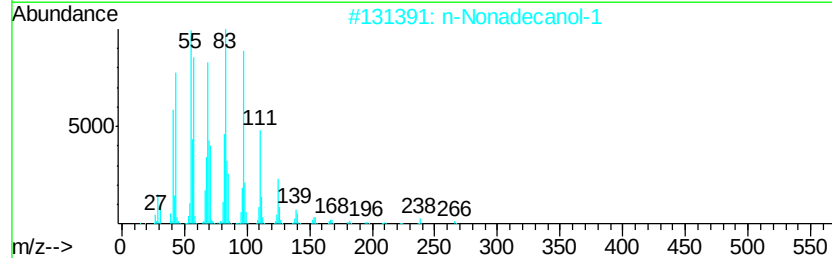
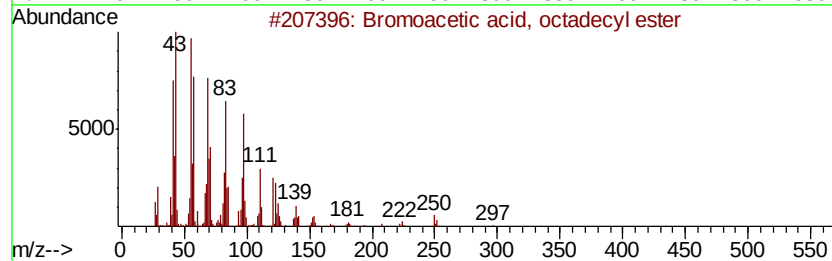
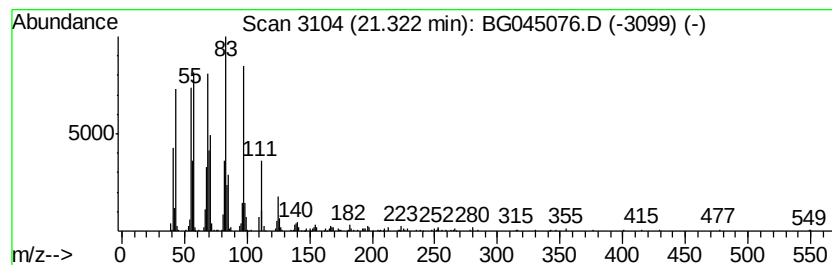
Instrument :
BNA_G
ClientSampleId :
DUP-2020-04-13

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 8 Bromoacetic acid, octadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.32	7.32 ng	455919	Chrysene-d12	21.66	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045076.D
Acq On : 18 Apr 2020 21:00
Operator : CG/JU
Sample : L2271-08
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-2020-04-13

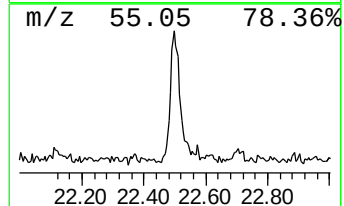
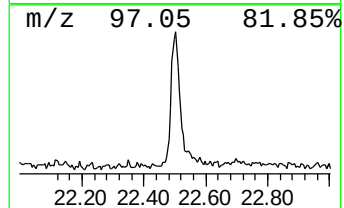
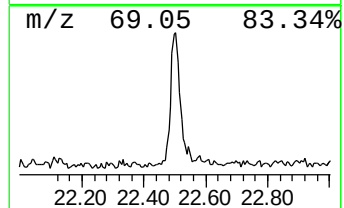
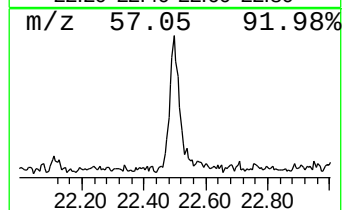
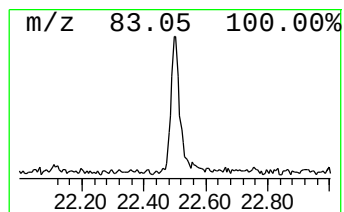
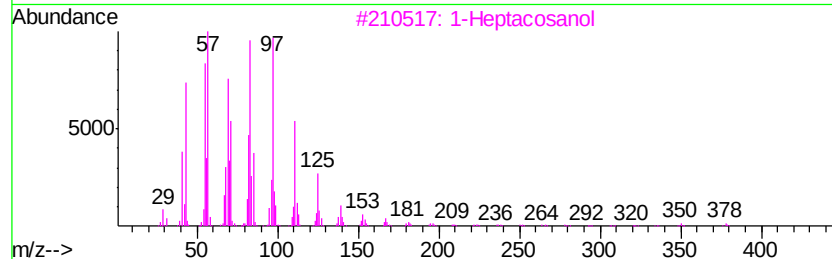
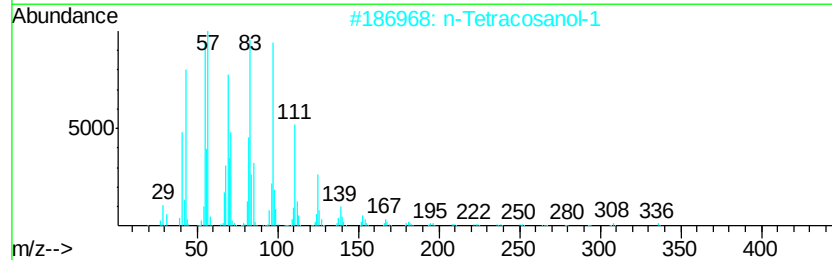
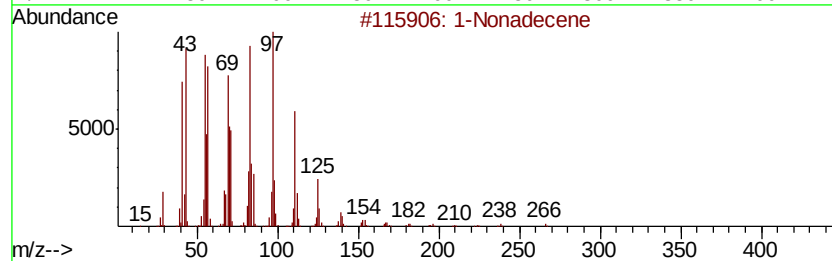
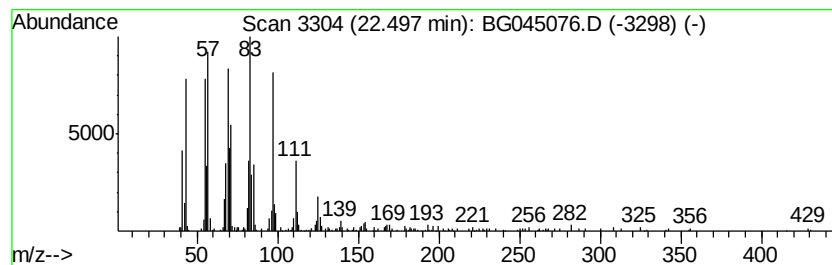
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.50	6.65 ng	413966	Chrysene-d12	21.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	92
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	91
3	1-Heptacosanol		396	C27H56O	002004-39-9	90
4	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	90
5	1-Docosene		308	C22H44	001599-67-3	89



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041720\
Data File : BG045076.D
Acq On : 18 Apr 2020 21:00
Operator : CG/JU
Sample : L2271-08
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-2020-04-13

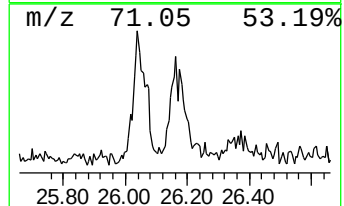
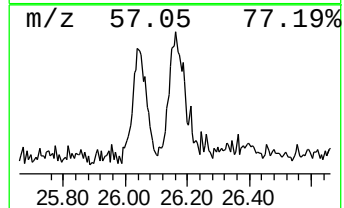
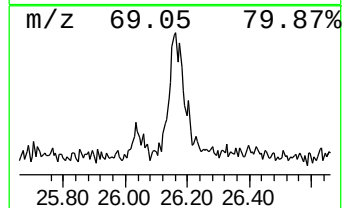
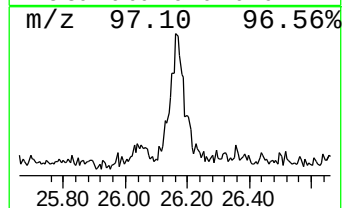
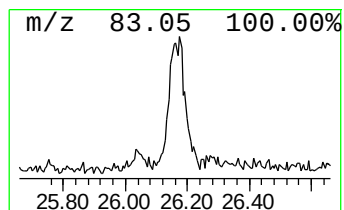
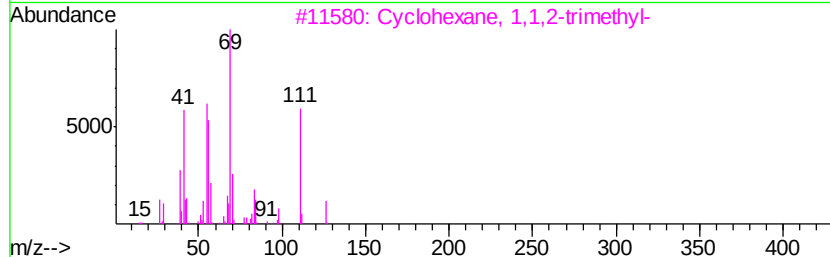
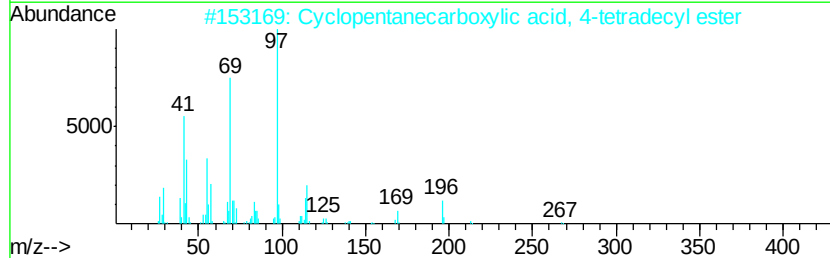
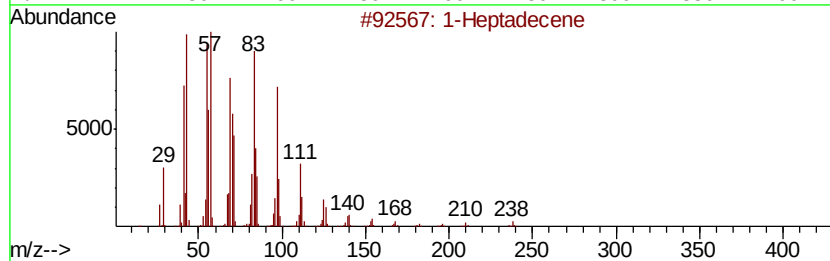
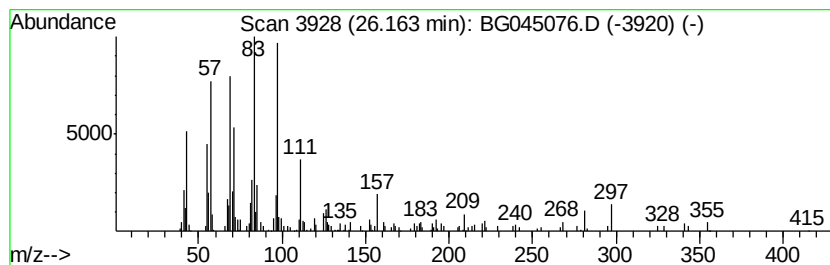
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heptadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.16	3.62 ng	214121	Perylene-d12	24.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptadecene	238	C17H34	006765-39-5	91
2		Cyclopentanecarboxylic acid, 4-t...	310	C20H38O2	1000280-58-9	38
3		Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	35
4		Cyclopentane, 1-butyl-2-propyl-	168	C12H24	062199-50-2	20
5		Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-26-2	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG041720\
Data File : BG045076.D
Acq On : 18 Apr 2020 21:00
Operator : CG/JU
Sample : L2271-08
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-2020-04-13

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	3.9	ng	71282	1	8.02	367511	20.0
(1R)-2,6,6-Trimet...	6.72	19.7	ng	361189	1	8.02	367511	20.0
.beta.-Pinene	7.47	3.9	ng	72043	1	8.02	367511	20.0
unknown20.69	20.69	2.1	ng	132378	5	21.66	1245250	20.0
Methyl dehydroabi...	20.75	2.8	ng	174215	5	21.66	1245250	20.0
Bromoacetic acid,...	21.32	7.3	ng	455919	5	21.66	1245250	20.0
1-Nonadecene	22.50	6.7	ng	413966	5	21.66	1245250	20.0
1-Heptadecene	26.16	3.6	ng	214121	6	24.85	1182130	20.0