

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG042020\
 Data File : BG045093.D
 Acq On : 20 Apr 2020 13:06
 Operator : CG/JU
 Sample : L2323-12
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-19-COMP

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	3.124	3	6	14	rVB	61415	105833	1.81%	0.353%
2	3.200	14	19	30	rVB	50960	85133	1.46%	0.284%
3	5.597	419	427	443	rBV	945854	1632314	27.91%	5.450%
4	7.195	690	699	709	rBV	1202688	2097312	35.86%	7.002%
5	8.023	834	840	848	rBV	239863	417856	7.14%	1.395%
6	8.346	888	895	904	rBV	972285	1781519	30.46%	5.948%
7	9.180	1030	1037	1048	rVB	836156	1545256	26.42%	5.159%
8	10.831	1310	1318	1324	rBV	347128	677326	11.58%	2.261%
9	13.280	1728	1735	1743	rBV	2616948	4209148	71.97%	14.053%
10	14.109	1868	1876	1881	rBV	486416	749080	12.81%	2.501%
11	14.655	1959	1969	1977	rBV	613353	1044270	17.86%	3.487%
12	16.147	2216	2223	2231	rBV	2246359	3419386	58.47%	11.417%
13	17.404	2430	2437	2442	rBV	780161	1275214	21.80%	4.258%
14	17.445	2442	2444	2450	rVB	94889	115801	1.98%	0.387%
15	19.454	2781	2786	2791	rVB	111275	160322	2.74%	0.535%
16	19.813	2842	2847	2856	rVB	128802	224940	3.85%	0.751%
17	20.018	2875	2882	2887	rBV	4311531	5848291	100.00%	19.526%
18	20.412	2945	2949	2953	rVB2	90889	116124	1.99%	0.388%
19	20.653	2985	2990	2994	rBV2	275503	391216	6.69%	1.306%
20	20.870	3025	3027	3034	rVB7	68234	83203	1.42%	0.278%
21	21.011	3047	3051	3056	rBV3	112926	150779	2.58%	0.503%
22	21.323	3100	3104	3109	rVB3	98152	144425	2.47%	0.482%
23	21.663	3155	3162	3168	rBV2	732594	1397093	23.89%	4.665%
24	22.321	3269	3274	3280	rBV2	144306	334603	5.72%	1.117%
25	22.462	3294	3298	3301	rBV	93778	151651	2.59%	0.506%
26	23.173	3415	3419	3426	rVB2	122255	226871	3.88%	0.757%
27	23.337	3442	3447	3457	rVB	119190	245131	4.19%	0.818%
28	24.565	3651	3656	3664	rVB2	58778	131148	2.24%	0.438%
29	24.859	3699	3706	3716	rBV2	421780	1189798	20.34%	3.972%

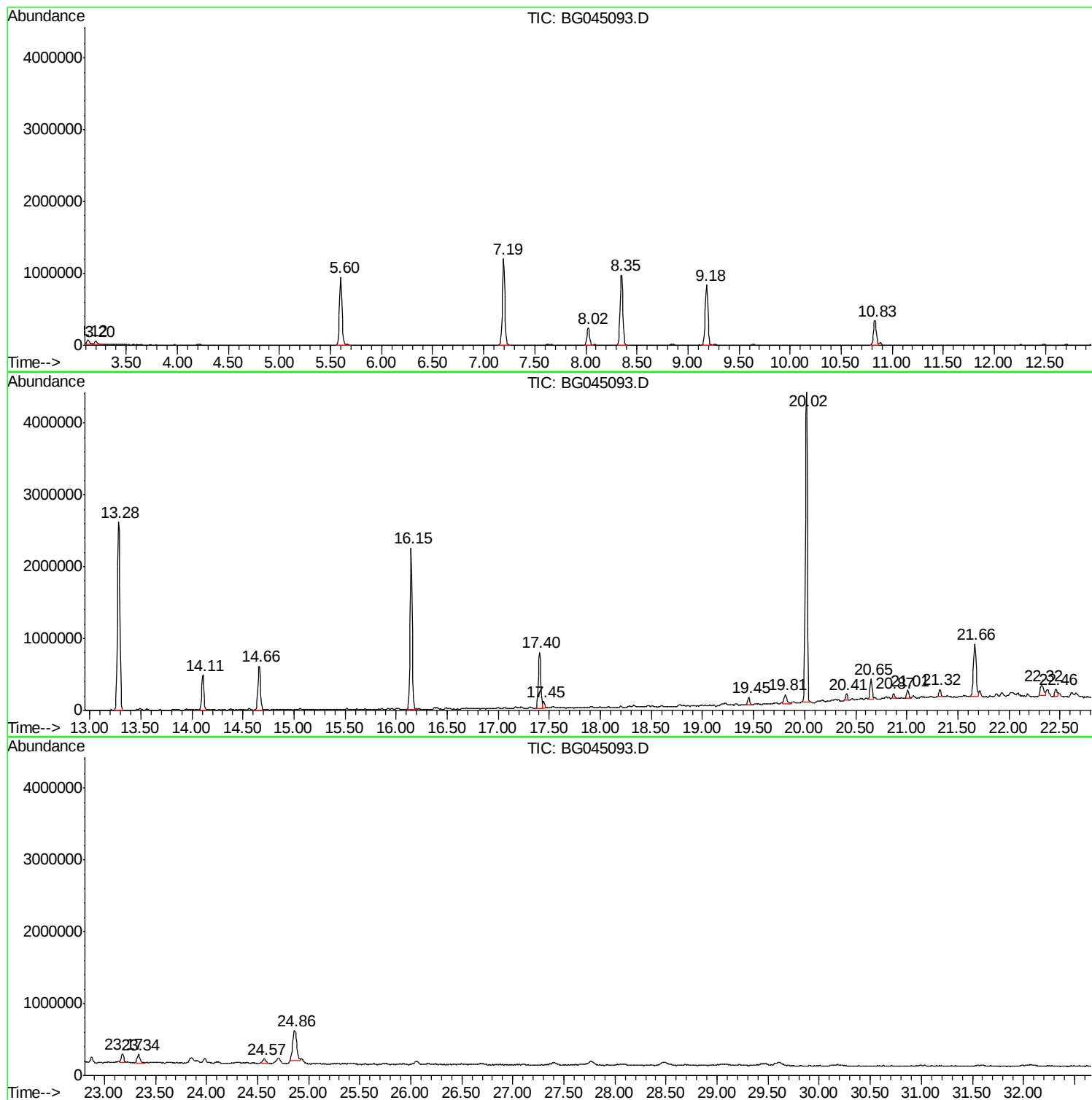
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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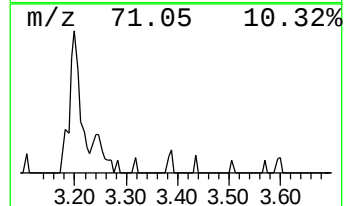
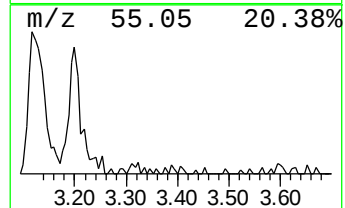
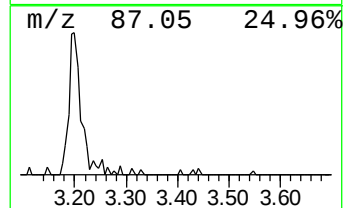
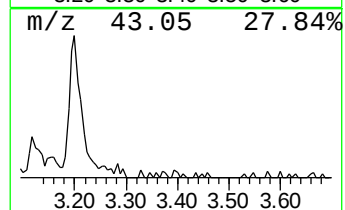
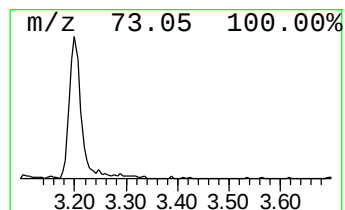
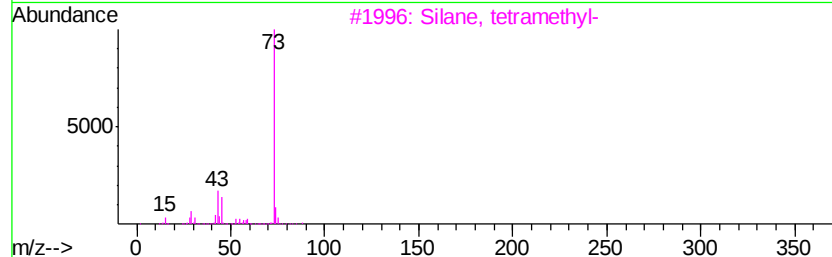
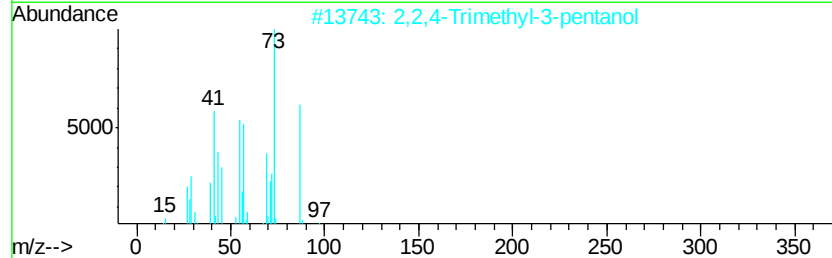
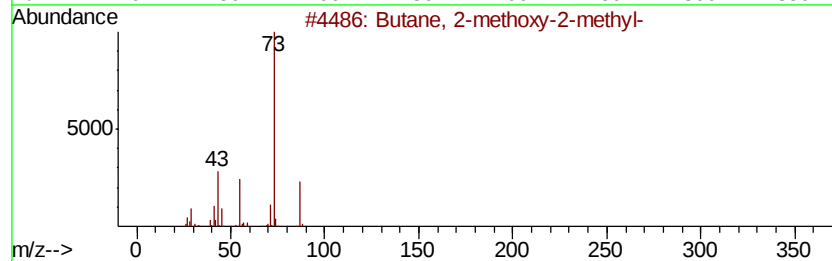
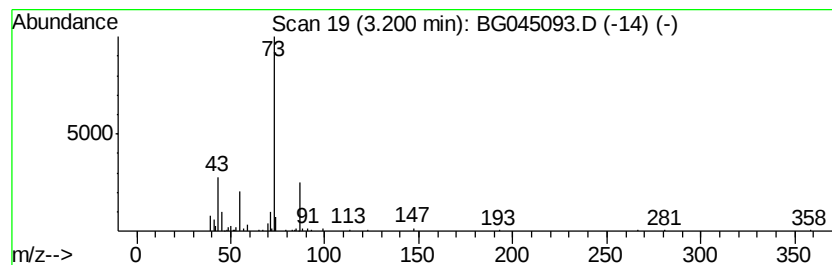
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	4.07 ng	85133	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	64
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		Silane, 2-hexenyltrimethyl-	156	C9H20Si	017898-20-3	10
5		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	10



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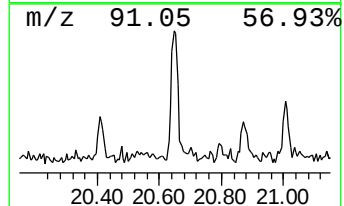
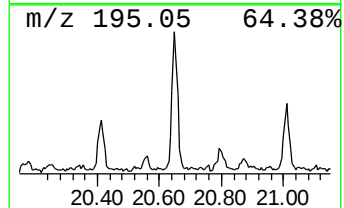
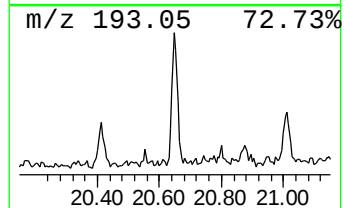
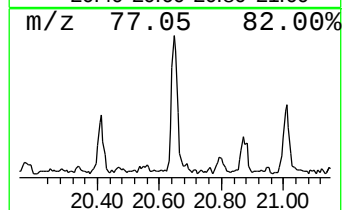
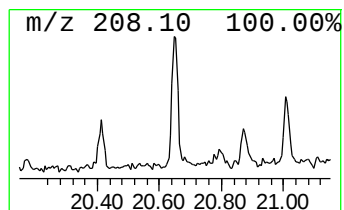
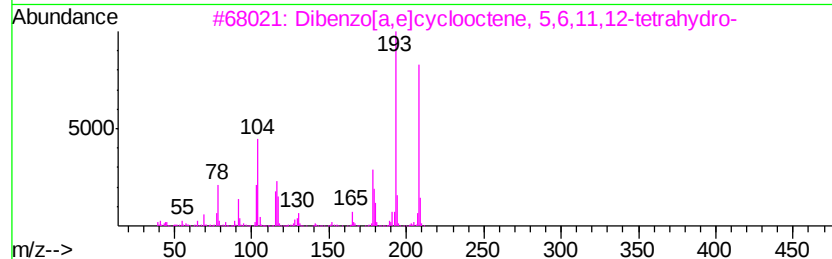
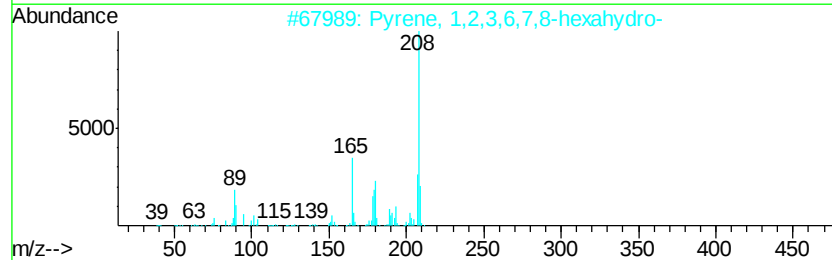
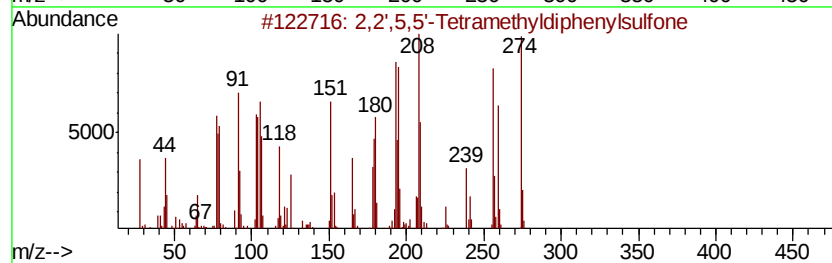
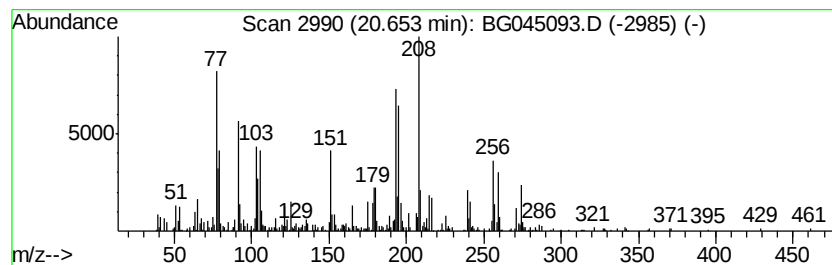
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Peak Number 5 2,2',5,5'-Tetramethyldiphen... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.65	5.60 ng	391216	Chrysene-d12	21.67	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2',5,5'-Tetramethyldiphenylsul...	274	C16H18O2S	006632-44-6	53
2	Pyrene, 1,2,3,6,7,8-hexahydro-	208	C16H16	001732-13-4	25
3	Dibenzo[a,e]lcvclooctene, 5,6,11,...	208	C16H16	001460-59-9	20
4	Isoelemicin	208	C12H16O3	000487-12-7	18
5	Naphthalene, 1,2,3,4-tetrahydro-...	208	C16H16	003018-20-0	15



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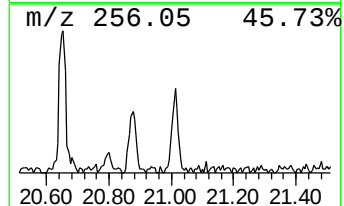
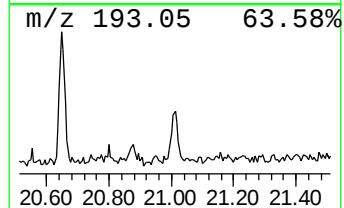
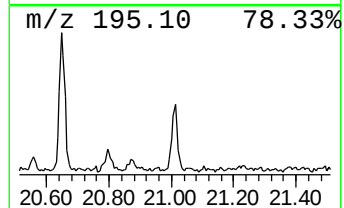
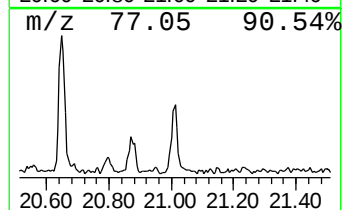
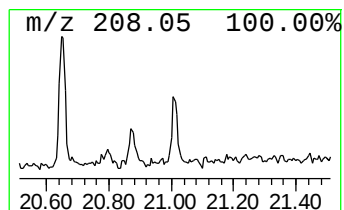
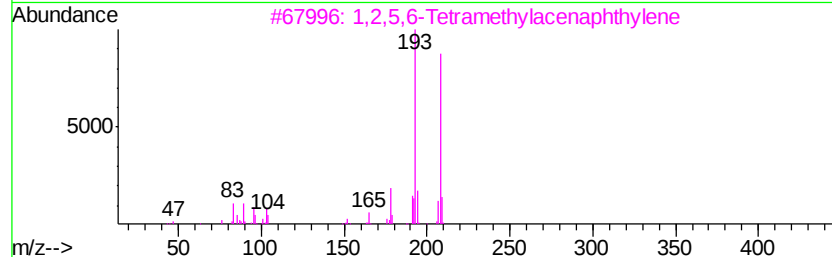
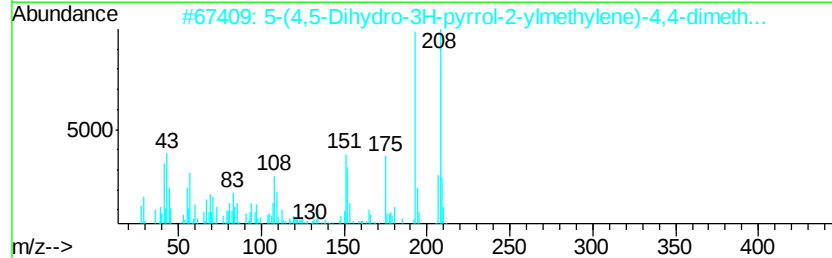
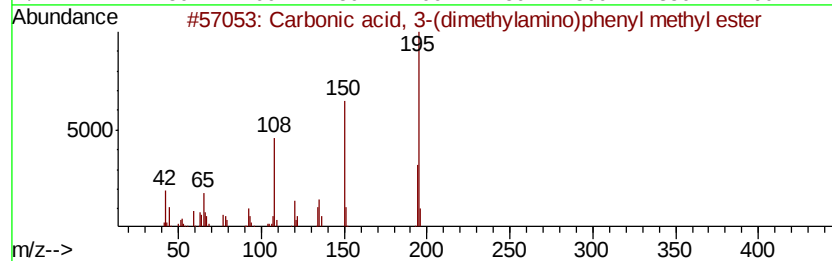
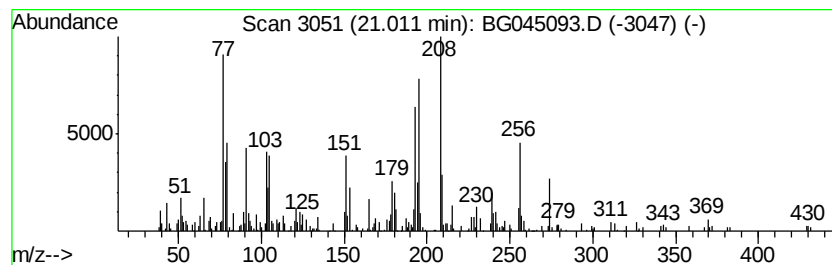
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Peak Number 6 unknown21.01 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.01	2.16 ng	150779	Chrysene-d12	21.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, 3-(dimethylamino)...	195	C10H13N03	054644-48-3	15
2		5-(4,5-Dihydro-3H-pyrrol-2-ylmet...	208	C11H16N2S	051430-88-7	14
3		1,2,5,6-Tetramethylacenaphthylene	208	C16H16	132118-73-1	14
4		2H-Benzotriazole, 5-nitro-2-phen...	256	C12H8N4O3	064264-32-0	14
5		Bis(2-methoxyphenyl) carbonate	274	C15H14O5	000553-17-3	11



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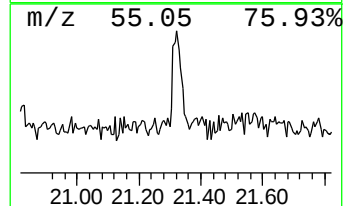
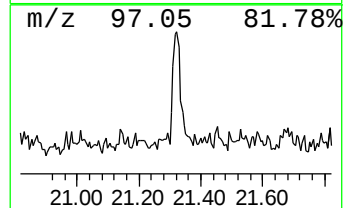
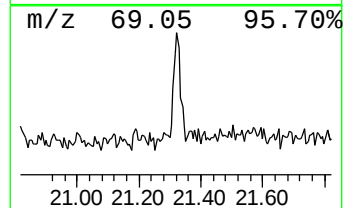
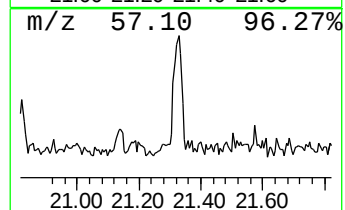
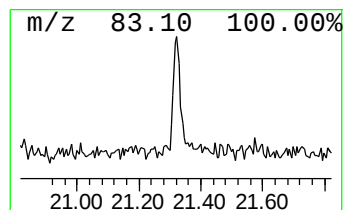
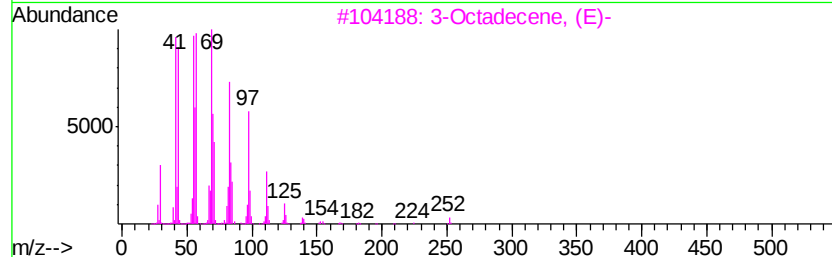
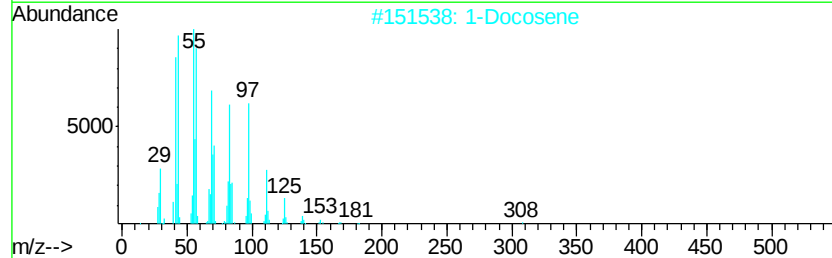
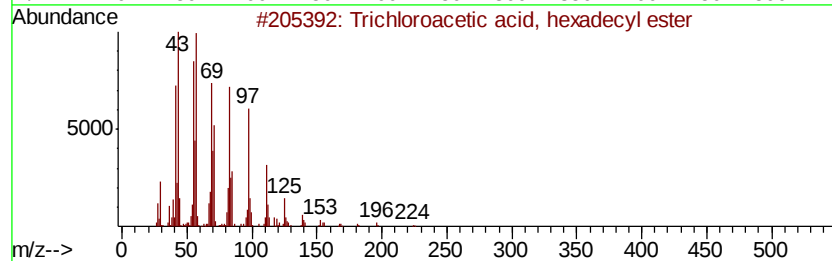
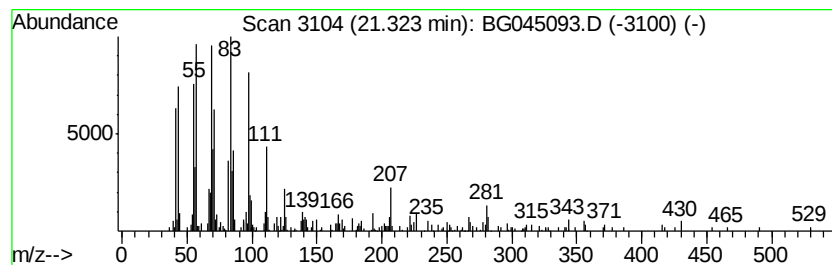
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Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	2.07 ng	144425	Chrysene-d12	21.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
2		1-Docosene	308	C22H44	001599-67-3	83
3		3-Octadecene, (E)-	252	C18H36	007206-19-1	83
4		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	81
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	76



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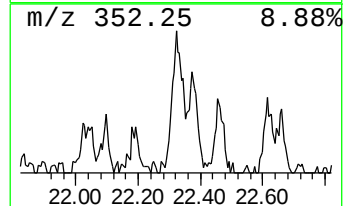
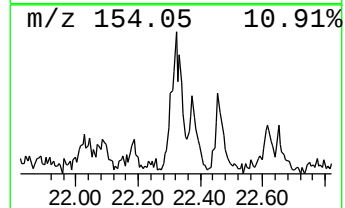
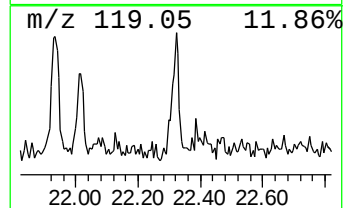
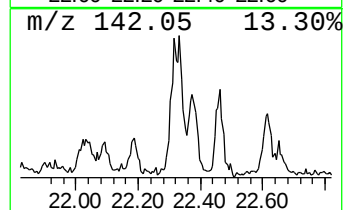
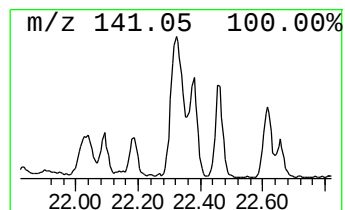
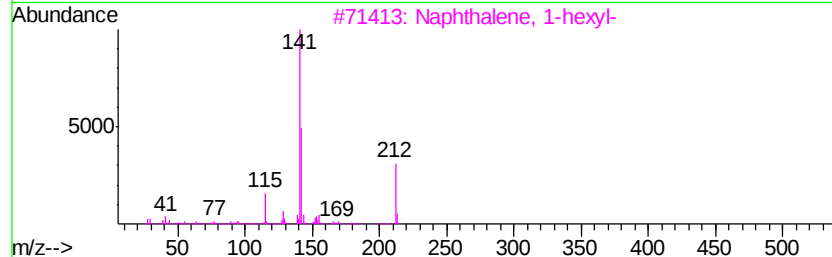
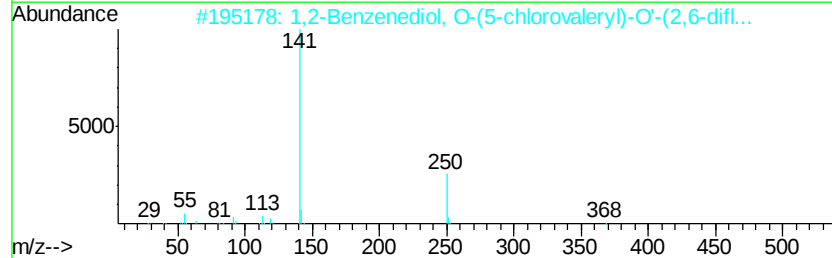
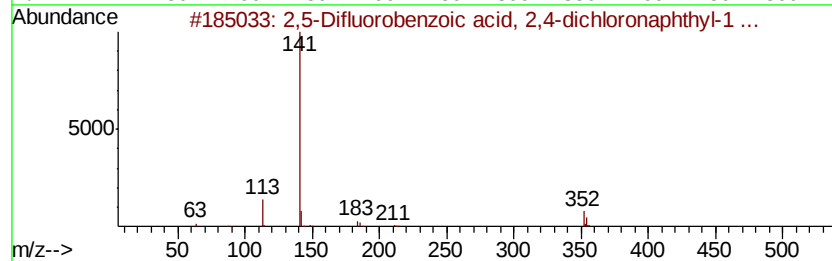
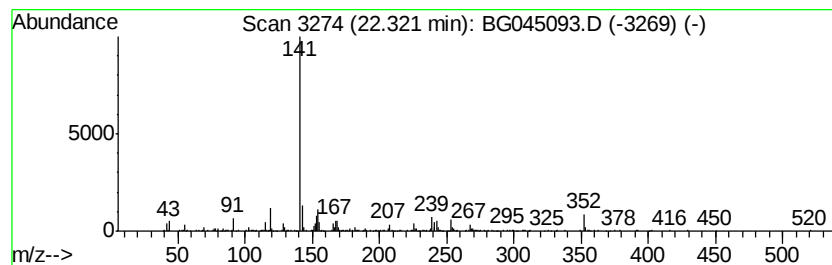
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Peak Number 8 2,5-Difluorobenzoic acid, 2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.32	4.79 ng	334603	Chrysene-d12	21.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Difluorobenzoic acid, 2,4-di...	352	C17H8Cl2F2O2	1000331-56-9	58
2		1,2-Benzenediol, O-(5-chlorovale...	368	C18H15ClF2O4	1000329-73-9	53
3		Naphthalene, 1-hexyl-	212	C16H20	002876-53-1	47
4		2,4-Difluorobenzoic acid, 2,4-di...	352	C17H8Cl2F2O2	1000331-58-5	42
5		1-[5-Nitro-6-uracilyl]-2-[2-chlo...	293	C12H8ClN3O4	296798-53-3	38



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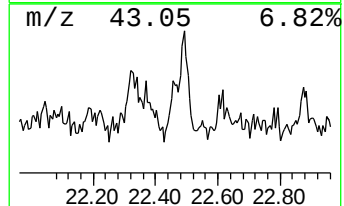
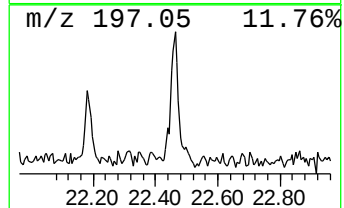
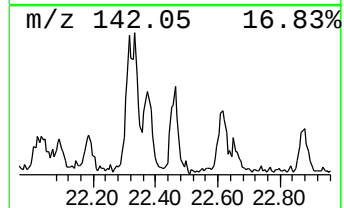
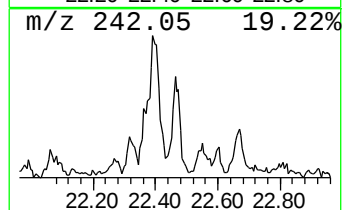
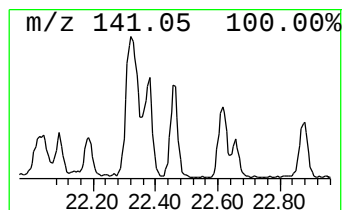
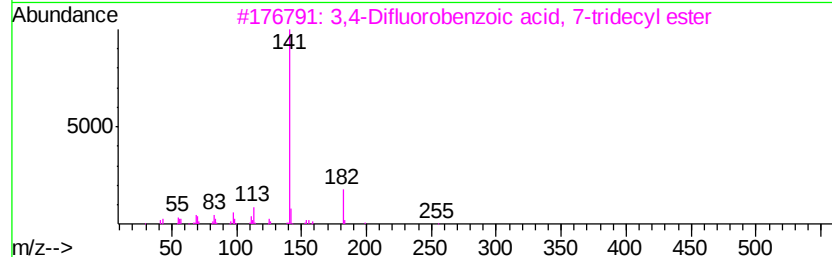
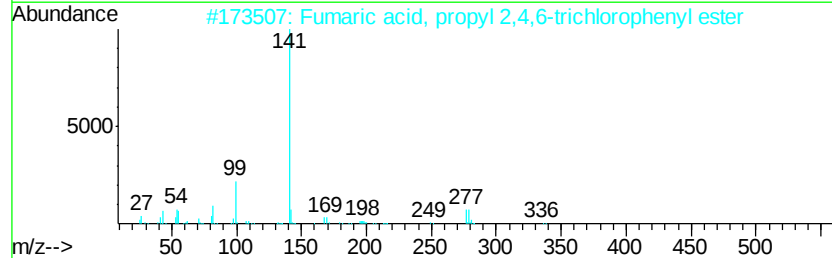
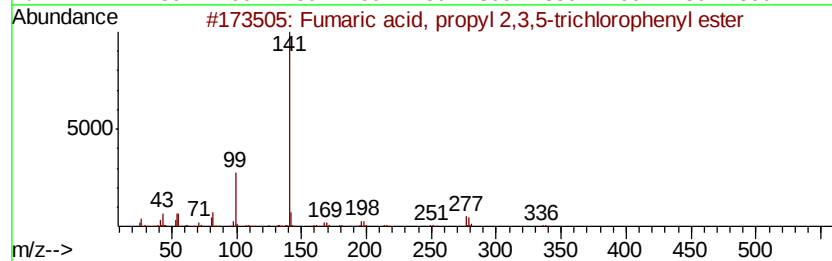
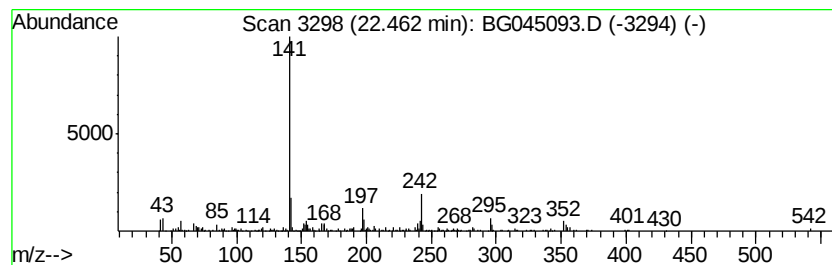
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown22.46 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.46	2.17 ng	151651	Chrysene-d12	21.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fumaric acid, propyl 2,3,5-trich...	336	C13H11Cl3O4	1000348-14-0	47
2		Fumaric acid, propyl 2,4,6-trich...	336	C13H11Cl3O4	1000348-26-8	47
3		3,4-Difluorobenzoic acid, 7-trid...	340	C20H30F2O2	1000338-60-4	47
4		Fumaric acid, 2,4-dimethylpent-3...	256	C14H24O4	1000348-54-2	42
5		2,4-Difluorobenzoic acid, 7-pent...	368	C22H34F2O2	1000338-58-0	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG042020\
Data File : BG045093.D
Acq On : 20 Apr 2020 13:06
Operator : CG/JU
Sample : L2323-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-19-COMP

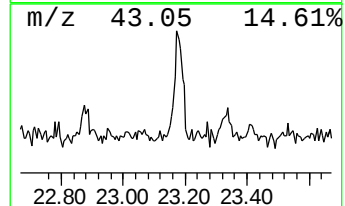
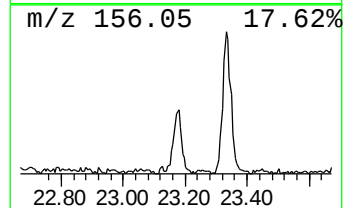
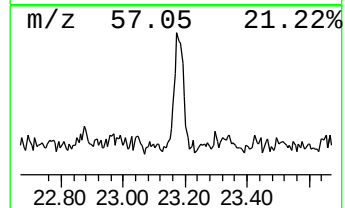
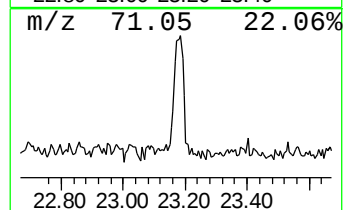
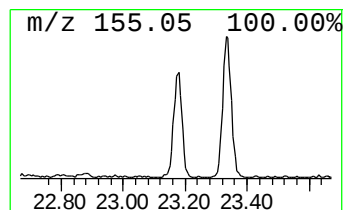
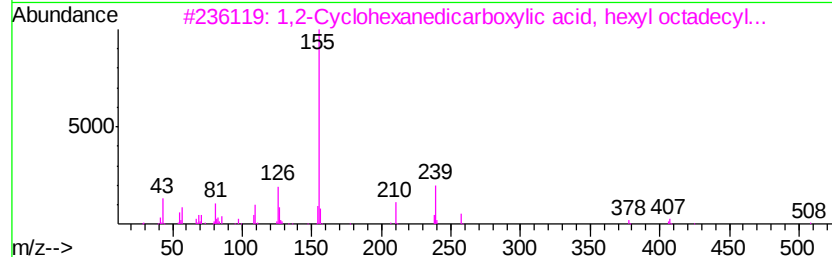
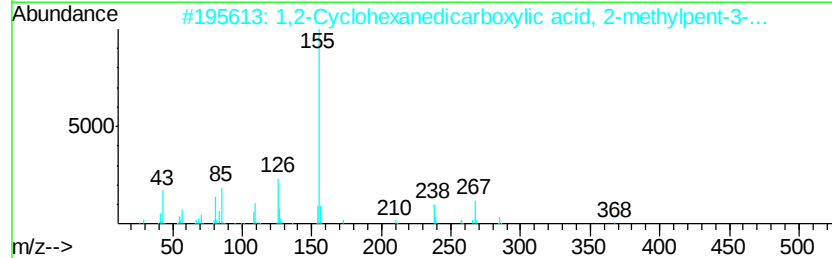
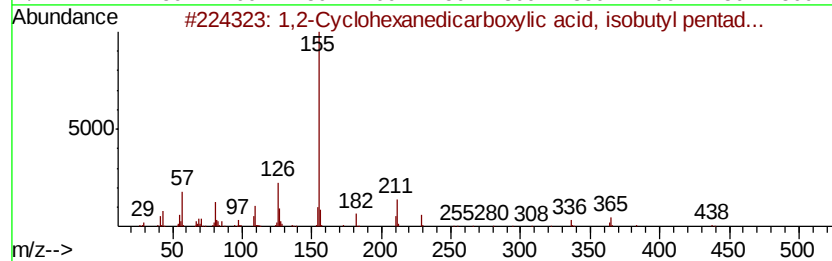
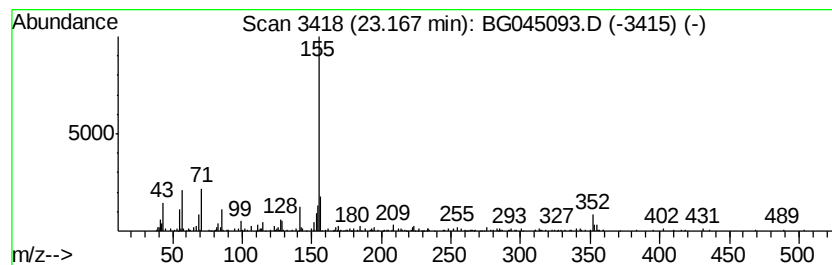
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,2-Cyclohexanedicarboxylic... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.17	3.25 ng	226871	Chrysene-d12	21.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Cyclohexanedicarboxylic acid...	438	C27H50O4	1000339-43-5	50
2		1,2-Cyclohexanedicarboxylic acid...	368	C22H40O4	1000339-44-5	50
3		1,2-Cyclohexanedicarboxylic acid...	508	C32H60O4	1000339-42-1	50
4		Decanoic anhydride	326	C20H38O3	002082-76-0	45
5		1-Naphthoic acid, 2,6-dimethylno...	320	C22H24O2	1000308-82-5	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG042020\
Data File : BG045093.D
Acq On : 20 Apr 2020 13:06
Operator : CG/JU
Sample : L2323-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-19-COMP

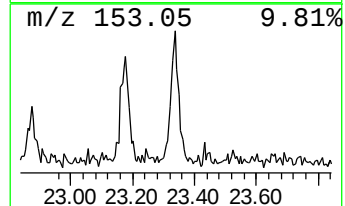
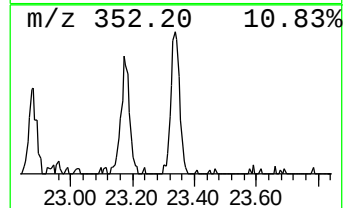
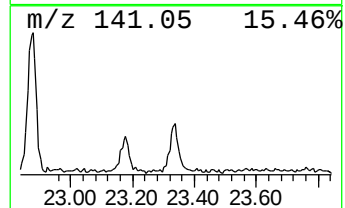
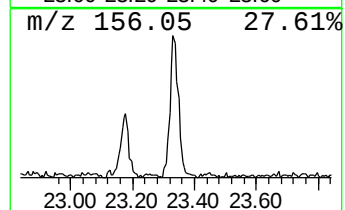
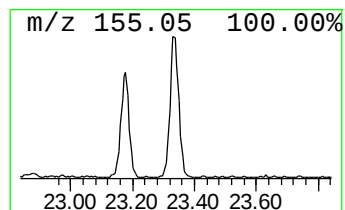
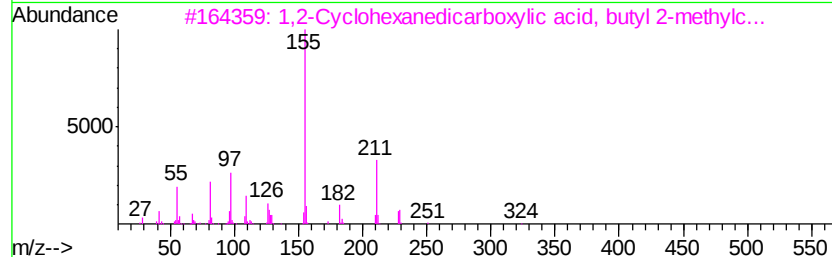
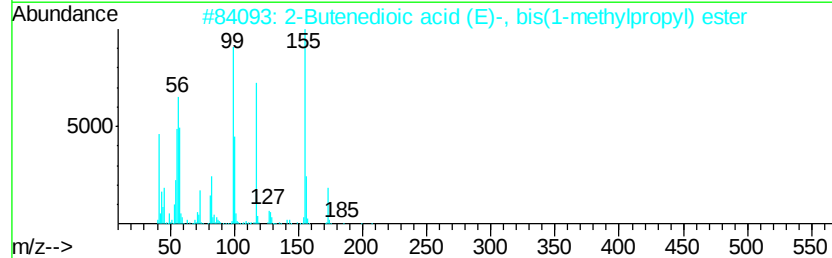
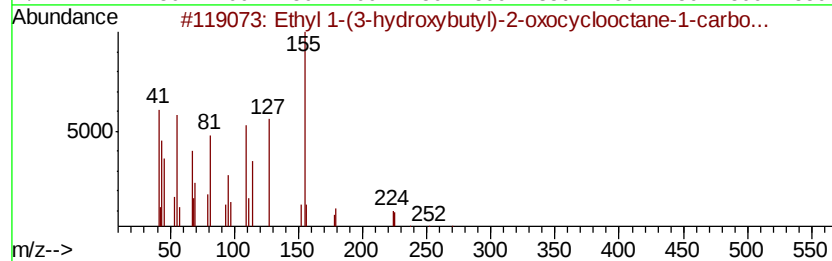
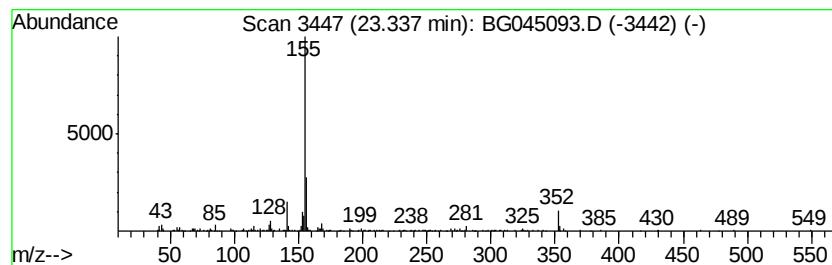
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG041520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown23.34 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.34	4.12 ng	245131	Perylene-d12	24.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl 1-(3-hydroxybutyl)-2-oxocyclooctane-1-carboxylate	270	C15H26O4	110288-16-9	47
2		2-Butenedioic acid (E)-, bis(1-methylpropyl) ester	228	C12H20O4	002210-32-4	42
3		1,2-Cyclohexanedicarboxylic acid, 1,2-bis(1-methylpropyl) ester	324	C19H32O4	1000339-87-7	38
4		Ethanone, 2-[5-(2-furyl)-1,3,4-oxadiazol-2-yl]propan-2-ol	336	C18H12N2O3S	296243-46-4	36
5		2-Tributylsilyloxybut-3-yne	268	C16H32OSi	1000299-53-9	28



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG042020\
Data File : BG045093.D
Acq On : 20 Apr 2020 13:06
Operator : CG/JU
Sample : L2323-12
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-19-COMP

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...	3.20	4.1 ng		85133	1	8.02	417856	20.0
2,2',5,5'-Tetrame...	20.65	5.6 ng		391216	5	21.67	1397090	20.0
unknown21.01	21.01	2.2 ng		150779	5	21.67	1397090	20.0
Trichloroacetic a...	21.32	2.1 ng		144425	5	21.67	1397090	20.0
2,5-Difluorobenzo...	22.32	4.8 ng		334603	5	21.67	1397090	20.0
unknown22.46	22.46	2.2 ng		151651	5	21.67	1397090	20.0
1,2-Cyclohexanedi...	23.17	3.3 ng		226871	5	21.67	1397090	20.0
unknown23.34	23.34	4.1 ng		245131	6	24.86	1189800	20.0