

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
 Data File : BG060190.D
 Acq On : 2 Jan 2024 11:49
 Operator : MA/JU
 Sample : 06039-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EC48-SOUTH

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

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

Signal : TIC: BG060190.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.113	3	4	10	rVB	255087	224597	1.56%	0.316%
2	5.041	325	332	342	rBV	236216	360323	2.50%	0.506%
3	5.511	405	412	424	rBV	3328463	5207329	36.10%	7.318%
4	5.922	477	482	490	rBV	195919	322209	2.23%	0.453%
5	7.103	673	683	696	rBV	3015168	5454582	37.82%	7.666%
6	7.937	817	825	836	rBV	570688	998798	6.92%	1.404%
7	9.101	1014	1023	1036	rBV	1628854	2958253	20.51%	4.157%
8	10.740	1295	1302	1314	rBV	809947	1497495	10.38%	2.105%
9	12.320	1563	1571	1579	rBV2	177627	374146	2.59%	0.526%
10	13.196	1712	1720	1730	rBV	5438352	8652343	59.99%	12.160%
11	14.024	1855	1861	1869	rBV	2120226	3109295	21.56%	4.370%
12	14.576	1946	1955	1962	rBV	1687628	2579361	17.88%	3.625%
13	15.370	2084	2090	2095	rBV	2798122	3679261	25.51%	5.171%
14	15.417	2095	2098	2103	rVB	164663	211606	1.47%	0.297%
15	16.063	2200	2208	2224	rBV	4288921	6612060	45.84%	9.292%
16	16.280	2240	2245	2248	rBV	197223	283829	1.97%	0.399%
17	17.073	2376	2380	2385	rBV	195590	235621	1.63%	0.331%
18	17.326	2416	2423	2432	rBV	2265989	3509977	24.34%	4.933%
19	17.814	2502	2506	2512	rBV2	178675	218339	1.51%	0.307%
20	18.507	2620	2624	2629	rBV	147356	170333	1.18%	0.239%
21	19.136	2726	2731	2733	rBV3	200947	297857	2.07%	0.419%
22	19.947	2862	2869	2881	rVV	10396782	14423141	100.00%	20.270%
23	21.233	3083	3088	3100	rBV3	463719	804799	5.58%	1.131%
24	21.592	3142	3149	3159	rBV2	2302422	3953413	27.41%	5.556%
25	23.061	3391	3399	3407	rBV9	57631	169846	1.18%	0.239%
26	23.255	3426	3432	3440	rVB	142945	265797	1.84%	0.374%
27	24.764	3678	3689	3705	rBV2	1440759	4223019	29.28%	5.935%
28	26.950	4054	4061	4066	rBV7	68937	201378	1.40%	0.283%
29	27.132	4085	4092	4098	rBV10	54397	156950	1.09%	0.221%

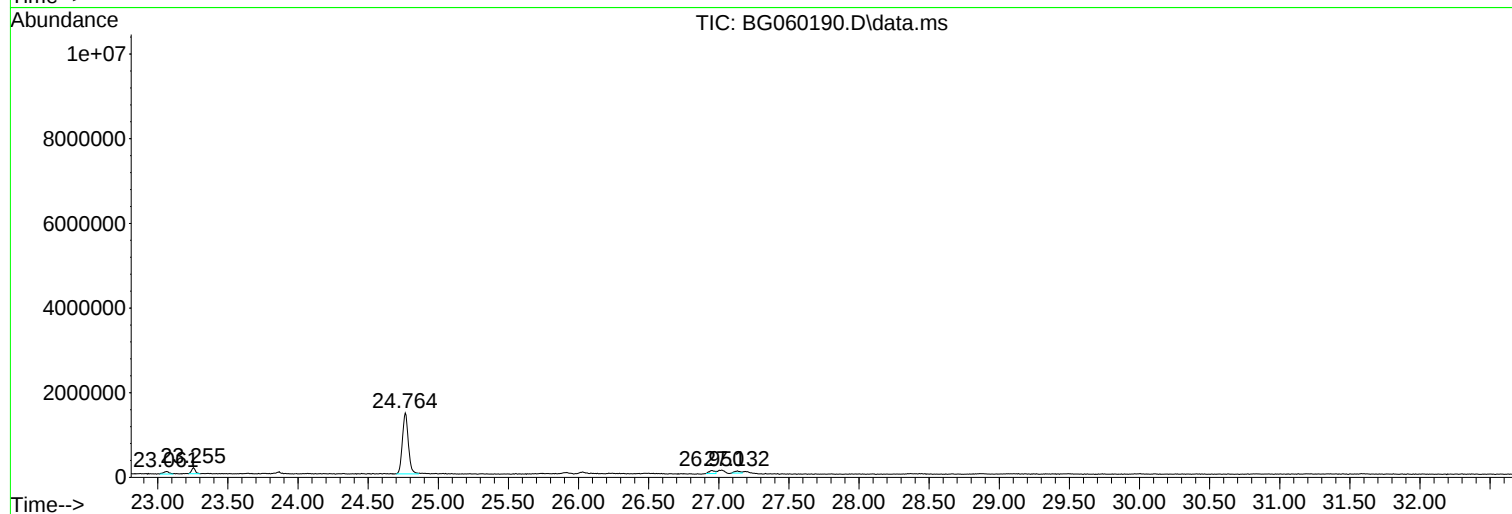
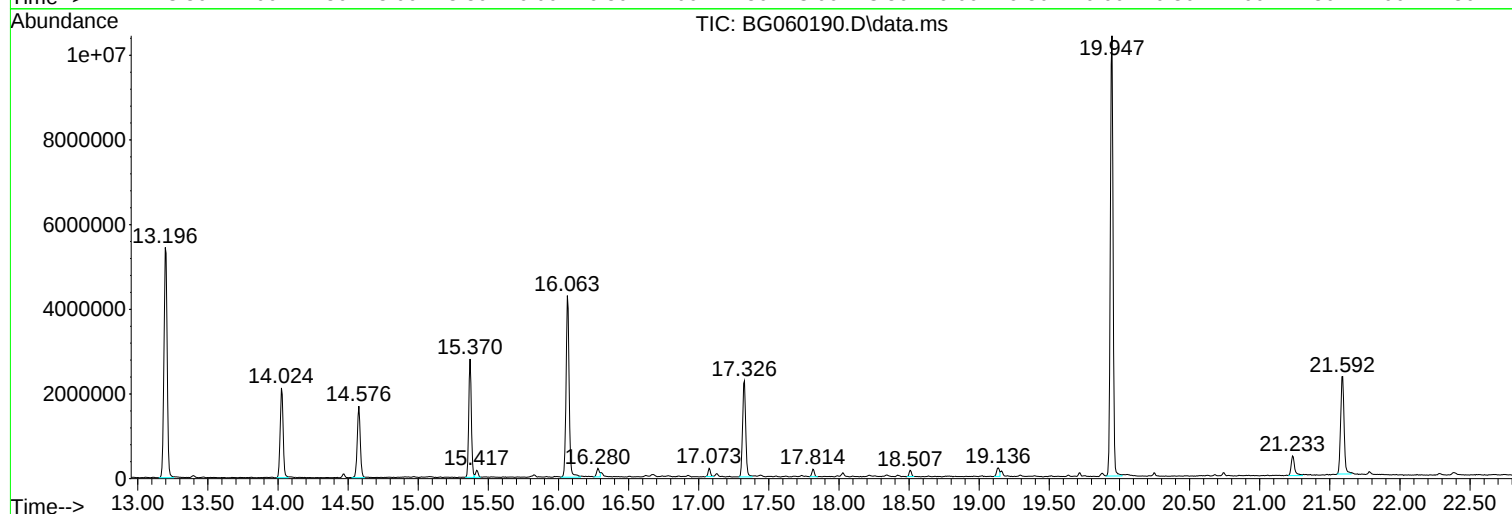
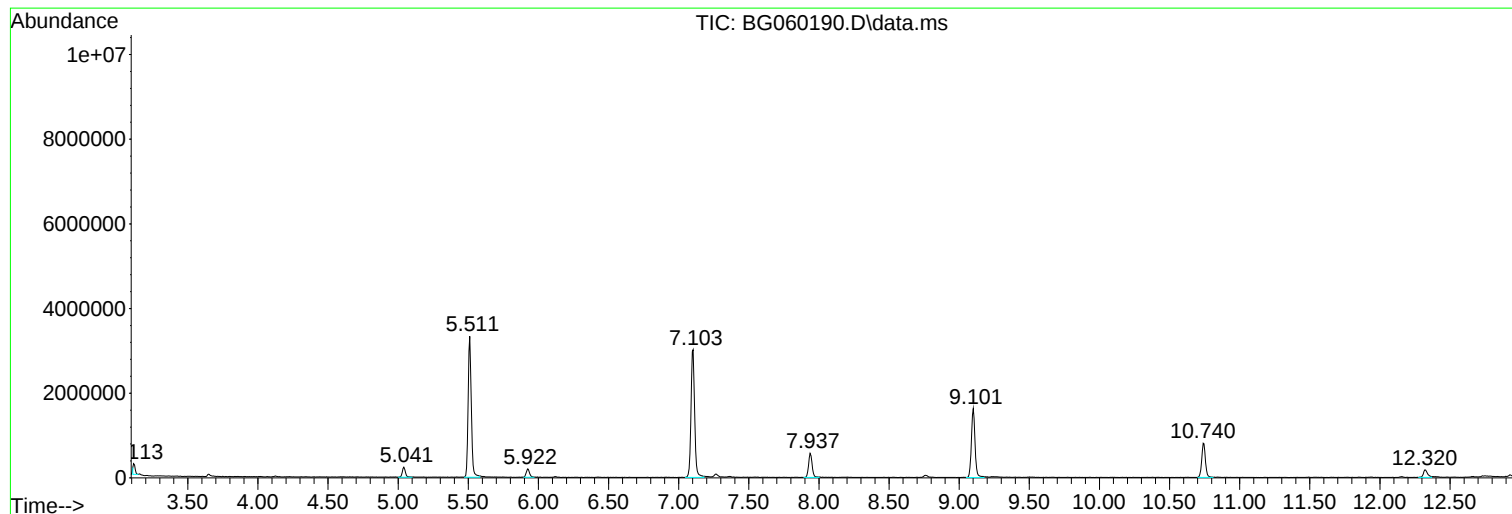
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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

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



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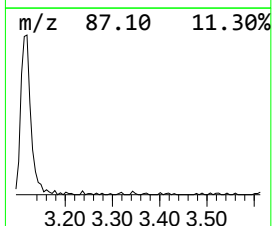
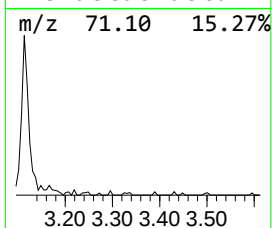
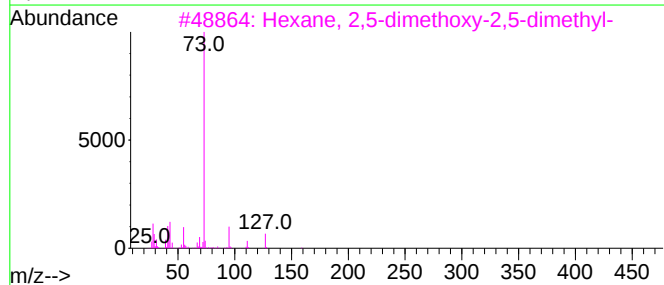
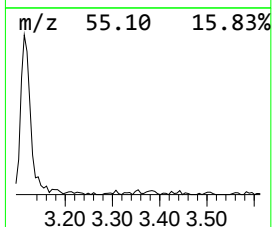
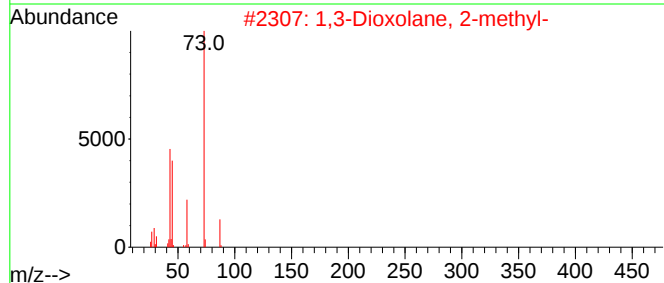
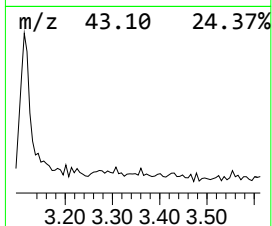
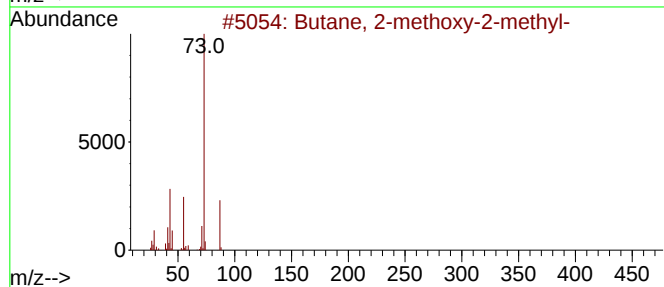
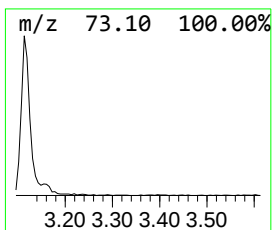
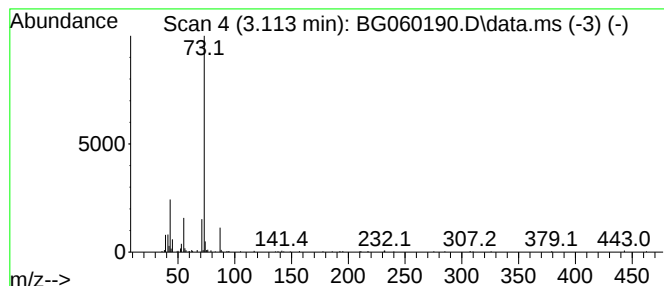
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.113	4.50 ng	224597	1,4-Dichlorobenzene-d4	7.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	53
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
3			Hexane, 2,5-dimethoxy-2,5-dimethyl-	174	C10H22O2	053273-13-5	9
4			Butane, 2,3-dimethoxy-2-methyl-	132	C7H16O2	074421-00-4	9
5			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	9



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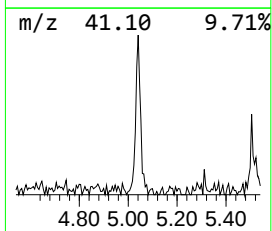
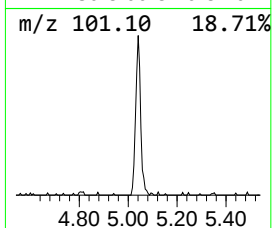
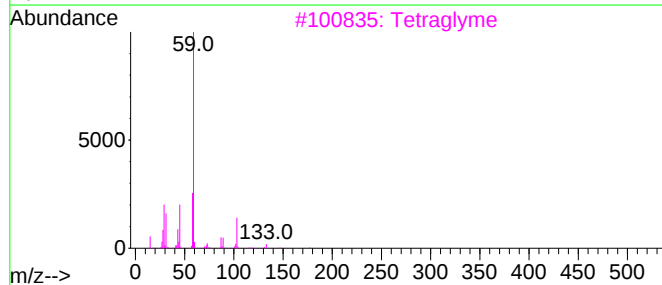
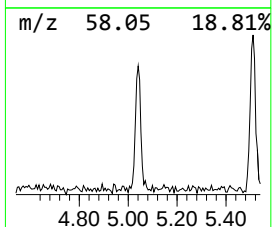
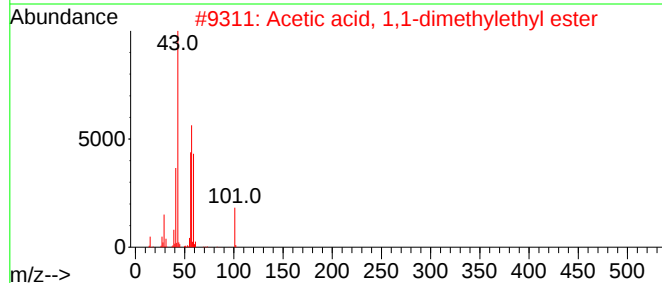
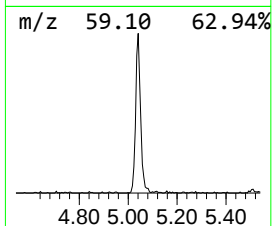
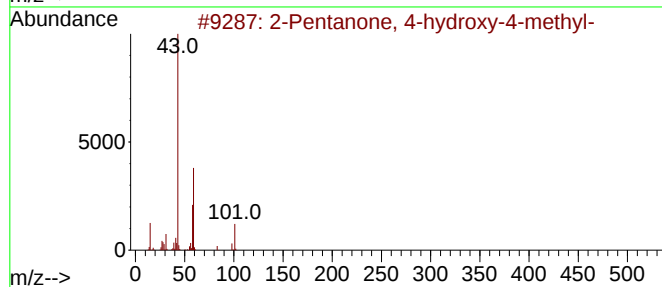
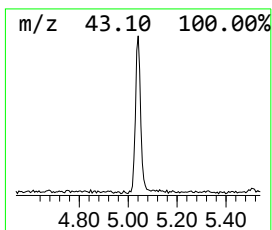
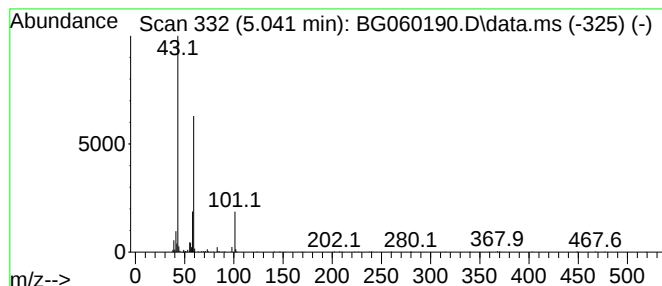
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.041	7.22 ng	360323	1,4-Dichlorobenzene-d4	7.937

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3			Tetraglyme	222	C10H22O5	000143-24-8	25
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	12



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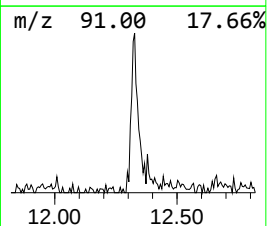
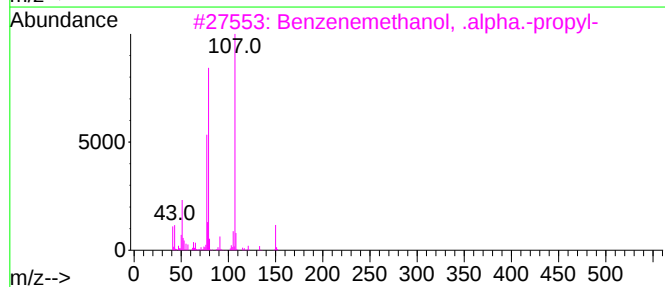
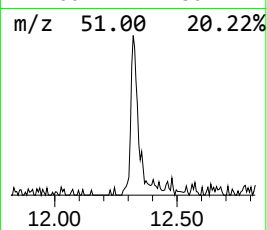
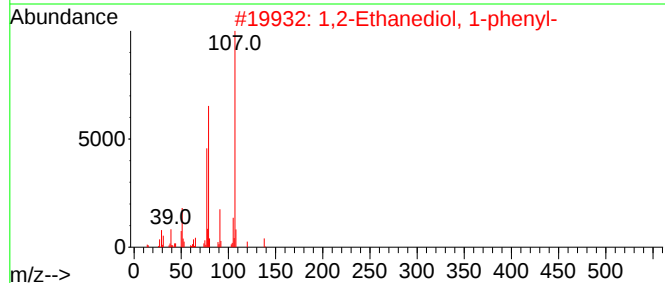
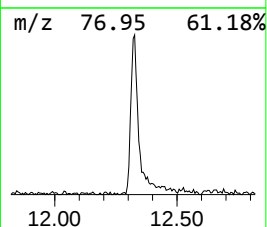
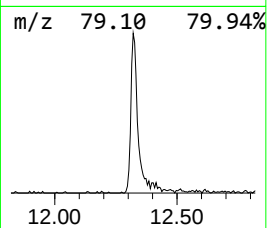
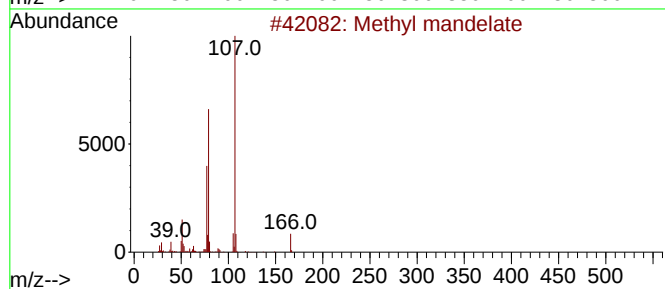
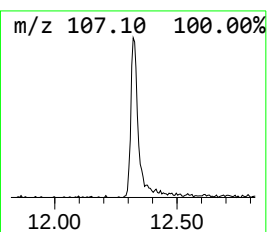
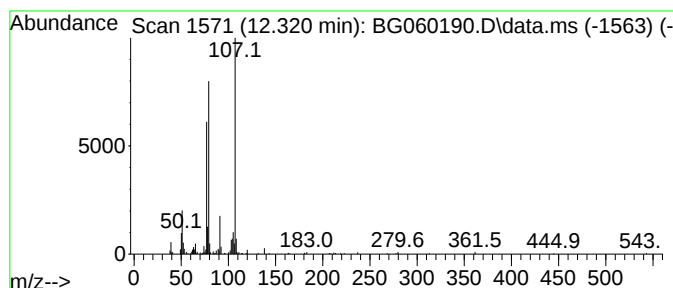
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Methyl mandelate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.320	5.00 ng	374146	Naphthalene-d8	10.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl mandelate	166	C9H10O3	004358-87-6	90
2			1,2-Ethanediol, 1-phenyl-	138	C8H10O2	000093-56-1	83
3			Benzenemethanol, .alpha.-propyl-	150	C10H14O	000614-14-2	83
4			Benzenemethanol, .alpha.-2-prope...	148	C10H12O	000936-58-3	83
5			Benzenemethanol, .alpha.-pentyl-	178	C12H18O	004471-05-0	78



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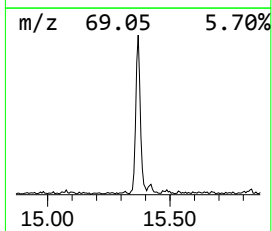
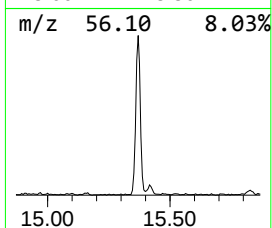
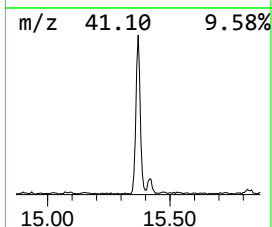
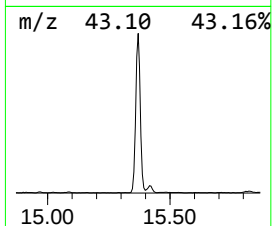
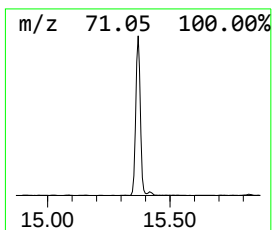
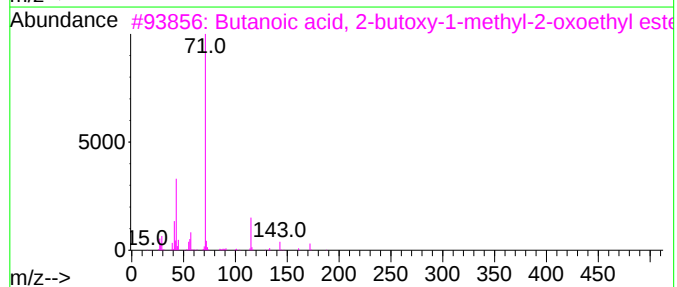
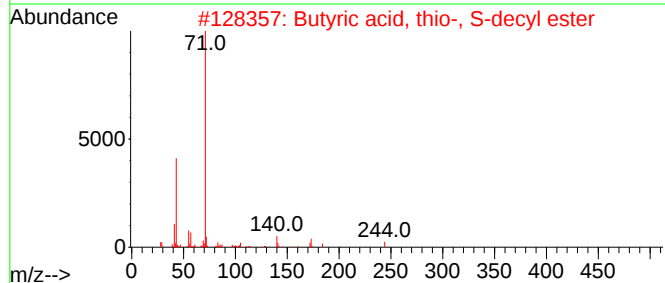
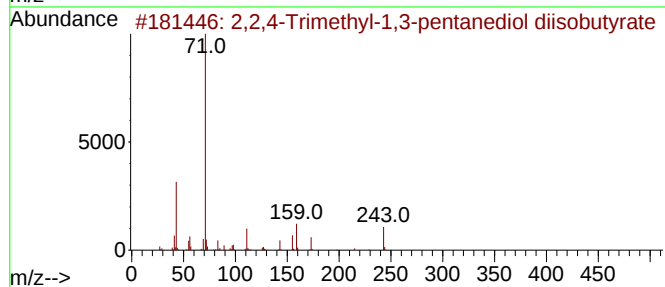
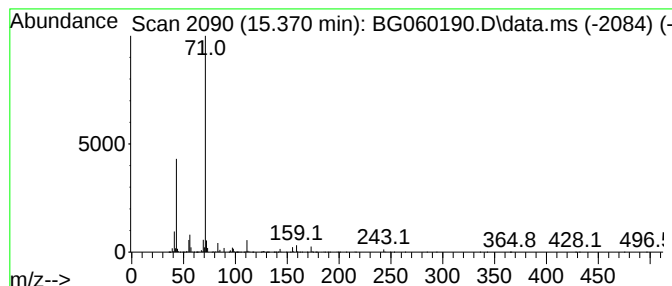
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.370	28.53 ng	3679260	Acenaphthene-d10	14.576	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	83
2	Butyric acid, thio-, S-decyl ester	244	C14H28OS	002432-55-5	50
3	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	50
4	Succinic acid, 2,2-dichloroethyl...	298	C11H16Cl2O5	1000390-71-6	50
5	Diethylmalonic acid, monochlorid...	262	C12H19ClO4	1000370-65-0	50



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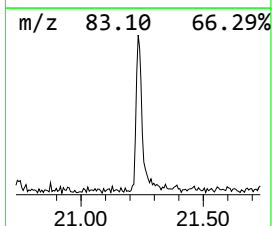
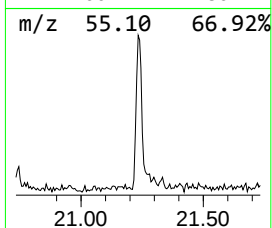
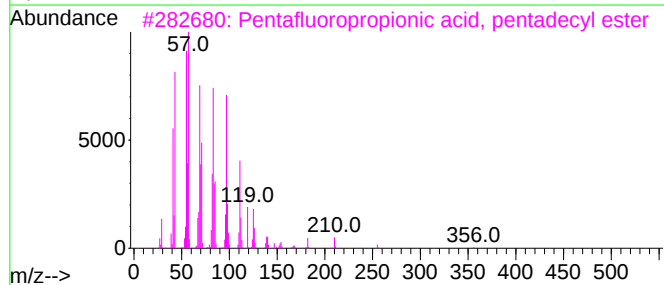
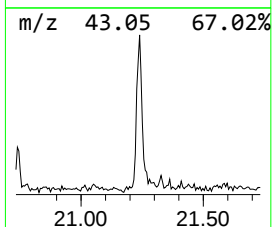
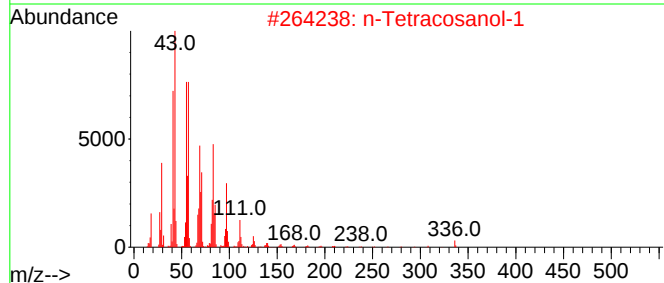
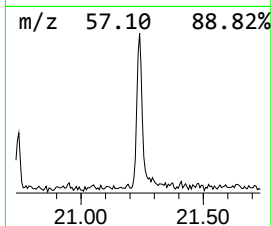
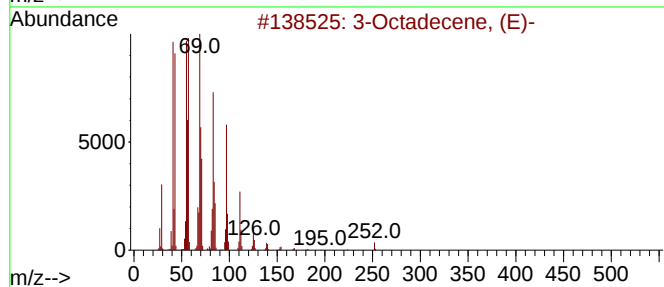
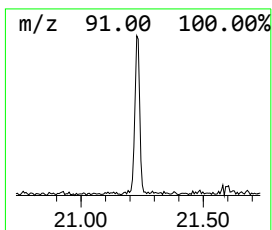
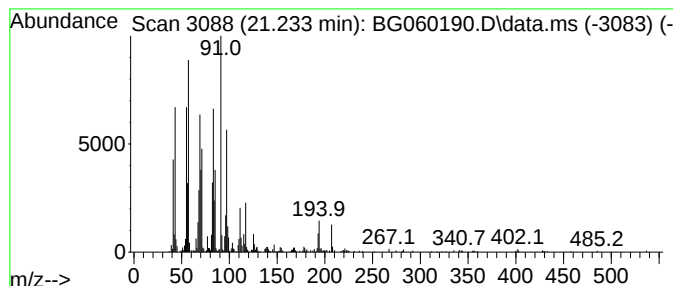
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Peak Number 6 3-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	4.07 ng	804799	Chrysene-d12	21.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octadecene, (E)-	252	C18H36	007206-19-1	96
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	83
4			1-Hexacosanol	382	C26H54O	000506-52-5	81
5			1-Octadecanol	270	C18H38O	000112-92-5	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.113	4.5	ng	224597	1	7.937	998798	20.0
2-Pentanone, 4-...	5.041	7.2	ng	360323	1	7.937	998798	20.0
Methyl mandelate	12.320	5.0	ng	374146	2	10.740	1497500	20.0
2,2,4-Trimethyl...	15.370	28.5	ng	3679260	3	14.576	2579360	20.0
3-Octadecene, (E)-	21.233	4.1	ng	804799	5	21.592	3953410	20.0