

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010821\
 Data File : BG047902.D
 Acq On : 9 Jan 2021 1:25
 Operator : CG/JU
 Sample : M1044-21
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-12

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-BG121720.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047902.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.508	24	29	34	rBV	55690	67985	1.33%	0.363%
2	4.707	228	233	239	rVB	92728	126461	2.46%	0.676%
3	5.177	307	313	316	rBV	56904	84208	1.64%	0.450%
4	5.747	402	410	420	rBV	810870	1417099	27.62%	7.573%
5	7.398	683	691	706	rBV	687650	1496992	29.18%	7.999%
6	7.744	743	750	759	rBV	29904	51732	1.01%	0.276%
7	8.161	813	821	828	rBV	174121	298256	5.81%	1.594%
8	9.331	1012	1020	1030	rVB	573646	1029181	20.06%	5.500%
9	10.987	1294	1302	1316	rVB	211852	393569	7.67%	2.103%
10	13.420	1708	1716	1724	rBV	1509500	2388568	46.56%	12.764%
11	13.673	1754	1759	1765	rBV	110002	173259	3.38%	0.926%
12	14.231	1848	1854	1861	rBV	120353	173274	3.38%	0.926%
13	14.795	1942	1950	1956	rBV2	366618	593983	11.58%	3.174%
14	16.281	2197	2203	2213	rBV	1573680	2400871	46.80%	12.829%
15	17.533	2408	2416	2422	rBV	557875	841591	16.40%	4.497%
16	20.124	2850	2857	2864	rBV	3884608	5130429	100.00%	27.415%
17	21.804	3136	3143	3152	rBV2	629556	1043901	20.35%	5.578%
18	25.136	3699	3710	3719	rBV2	352740	1002326	19.54%	5.356%

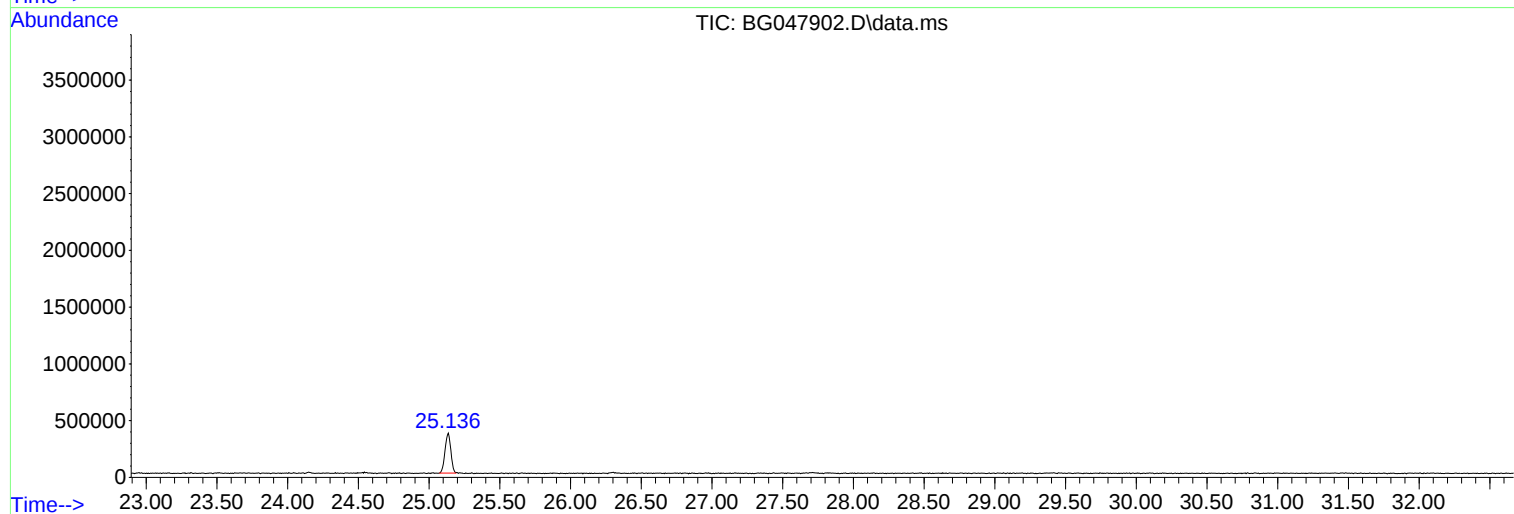
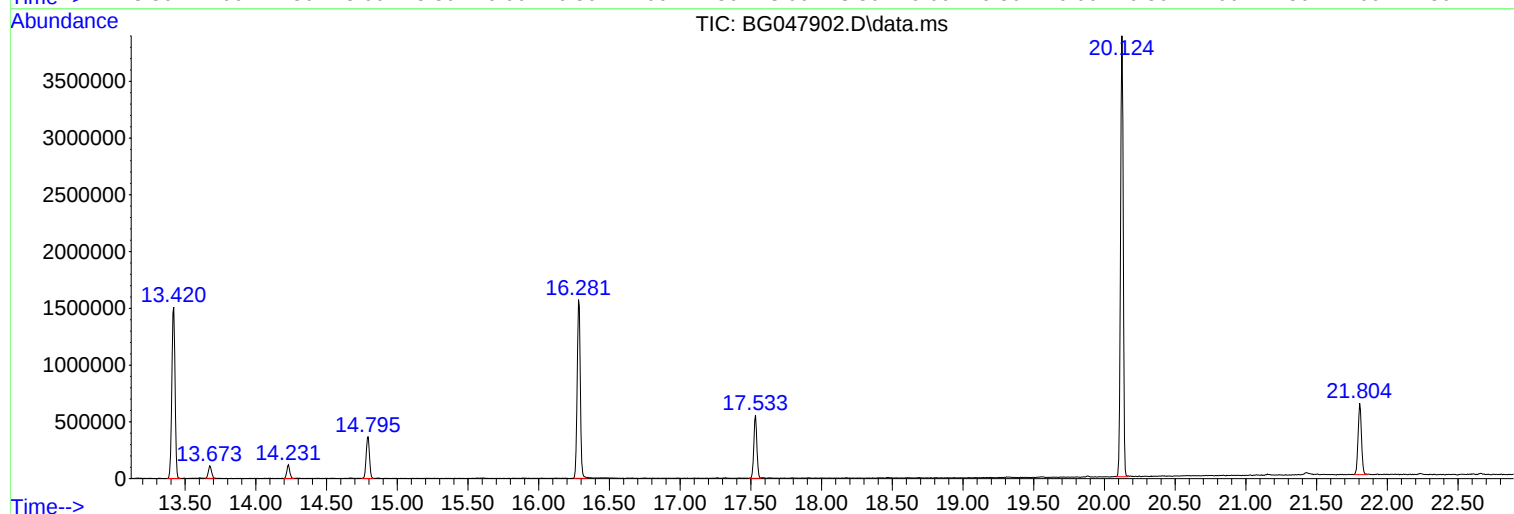
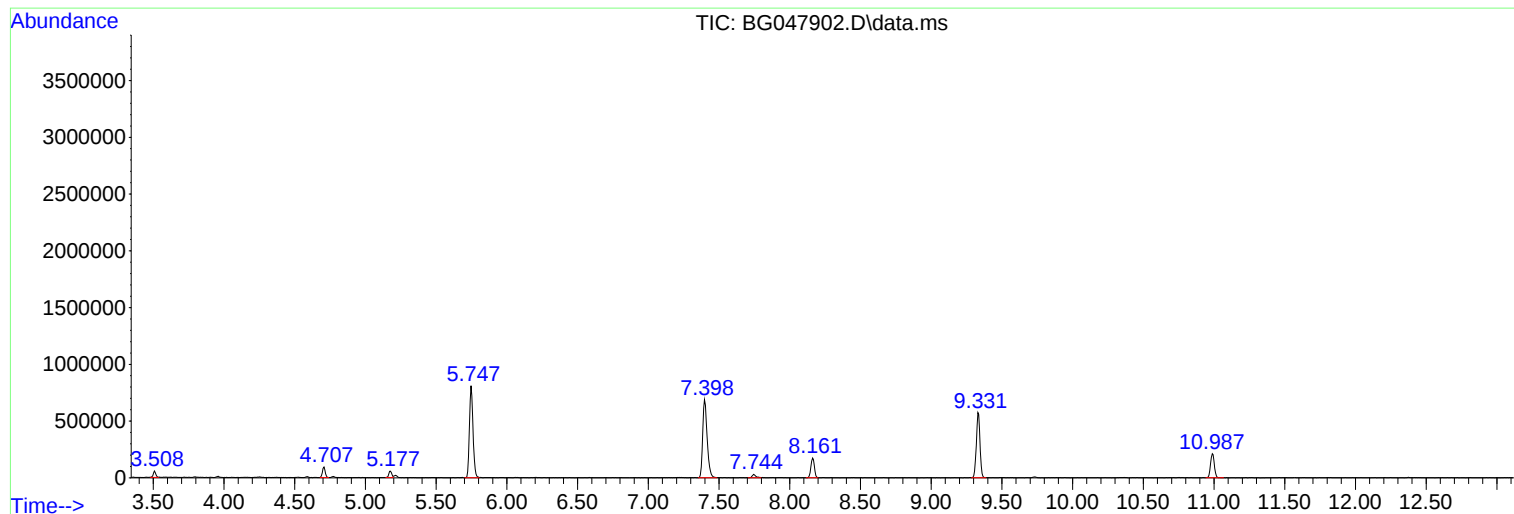
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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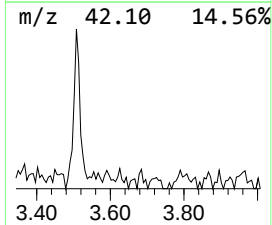
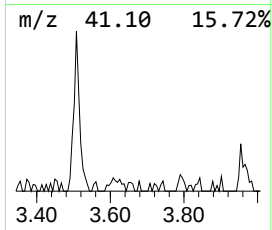
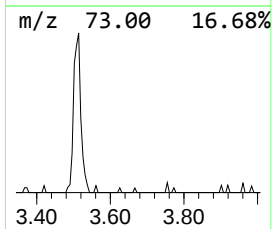
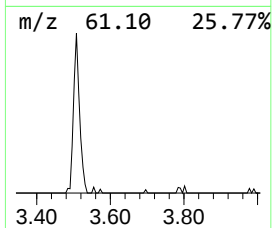
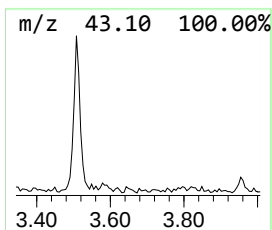
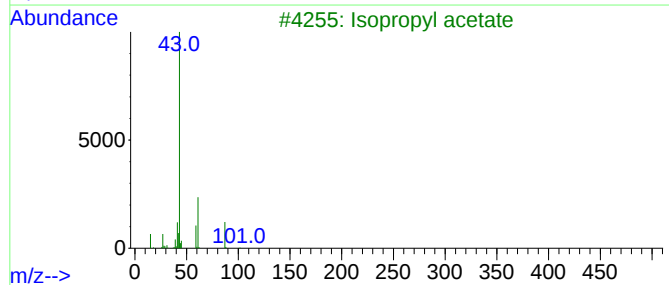
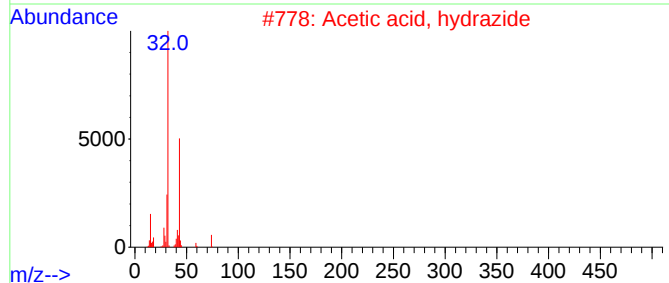
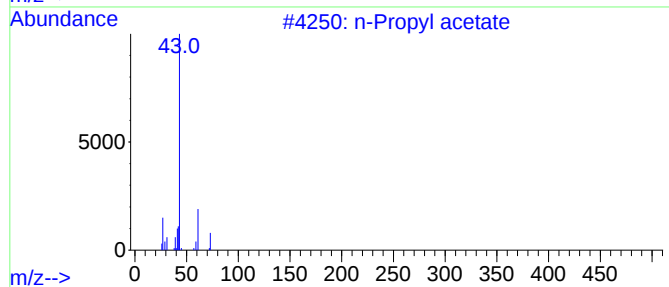
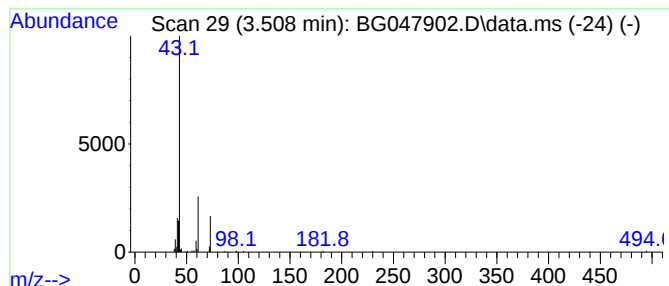
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.508	4.56 ng	67985	1,4-Dichlorobenzene-d4	8.161

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	50
2			Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	9
3			Isopropyl acetate	102	C5H10O2	000108-21-4	9
4			1-Pentanol, 5-chloro-, acetate	164	C7H13ClO2	020395-28-2	9
5			Isobutylamine	73	C4H11N	000078-81-9	7



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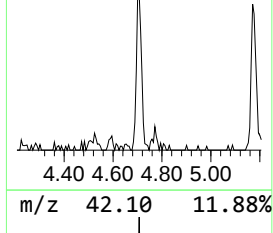
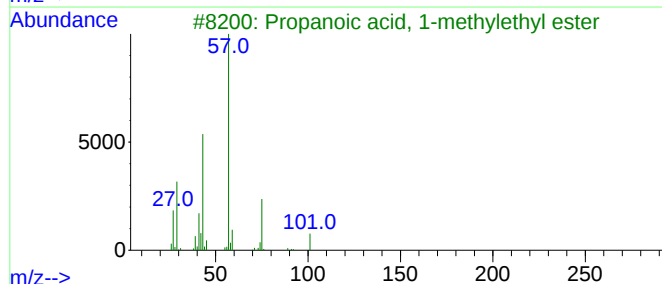
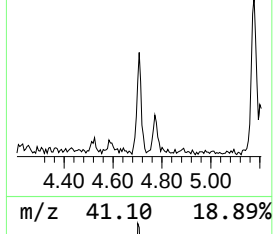
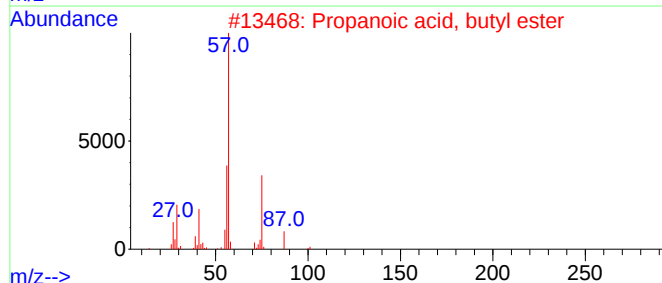
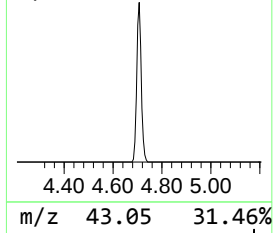
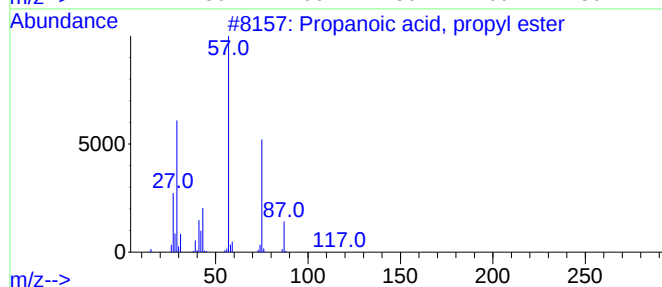
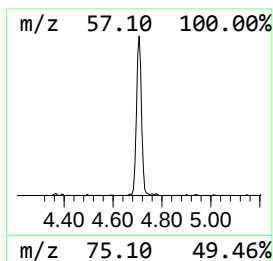
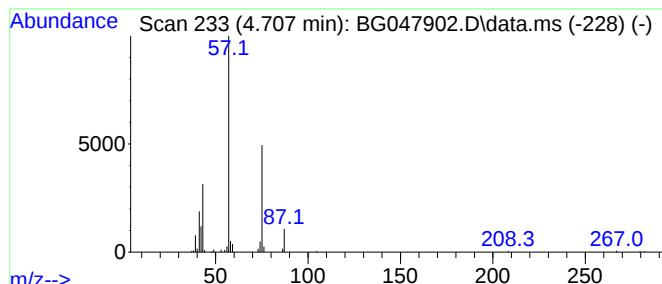
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.707	8.48 ng	126461	1,4-Dichlorobenzene-d4	8.161

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	17
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
5			1-Pentanamine	87	C5H13N	000110-58-7	9



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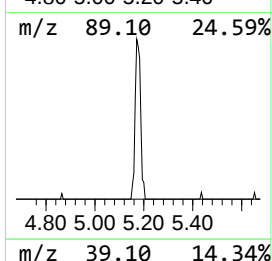
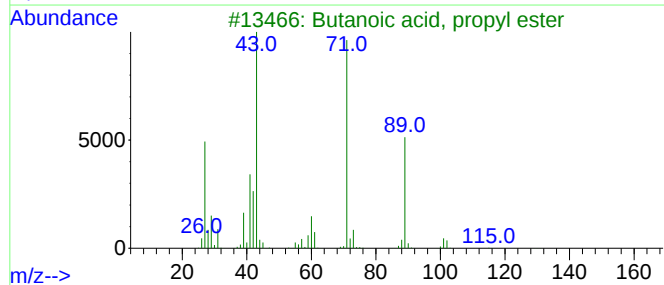
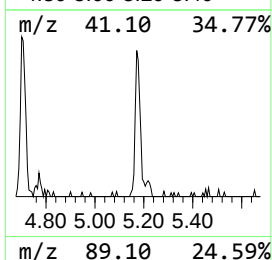
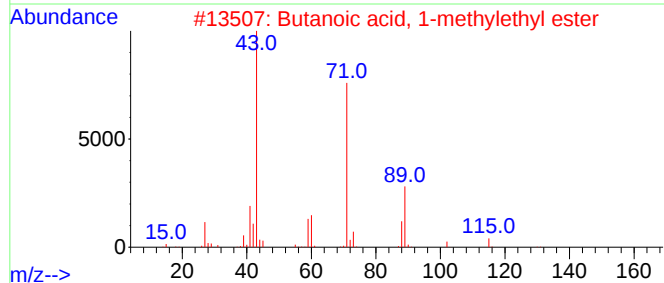
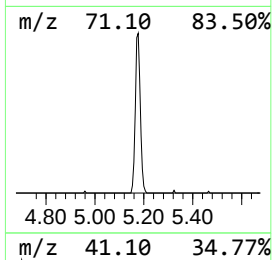
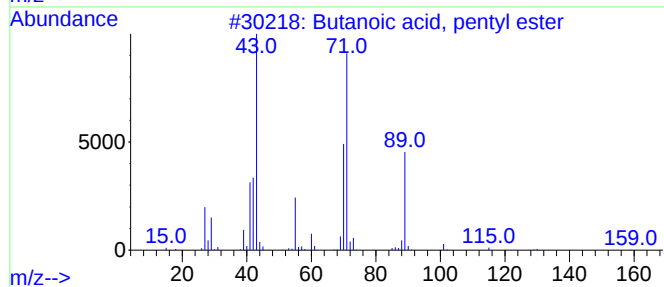
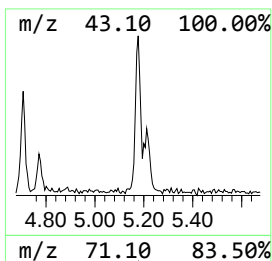
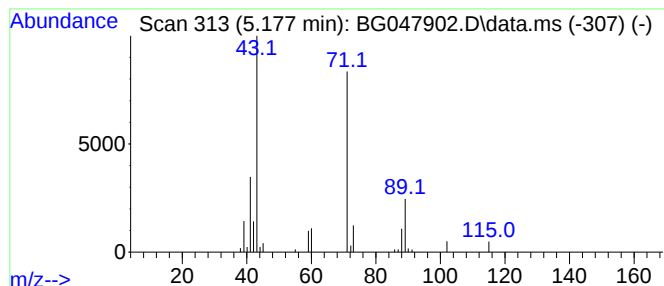
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Peak Number 3 Butanoic acid, pentyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.177	5.65 ng	84208	1,4-Dichlorobenzene-d4	8.161

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	59
2			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	53
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42
4			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	36
5			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	33



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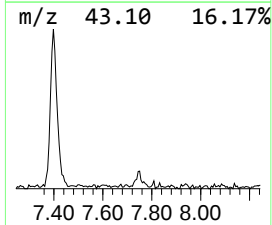
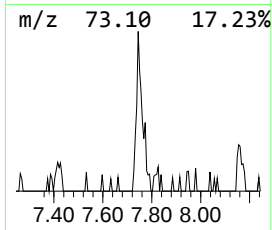
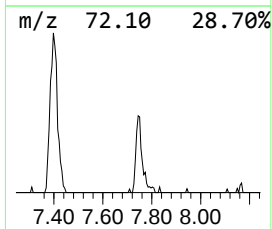
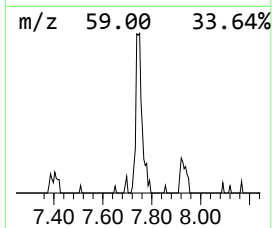
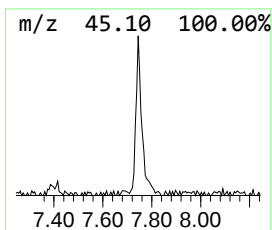
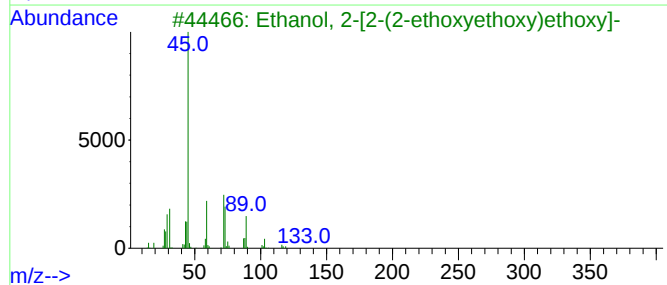
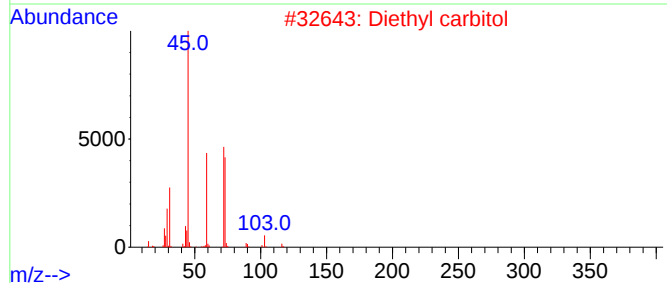
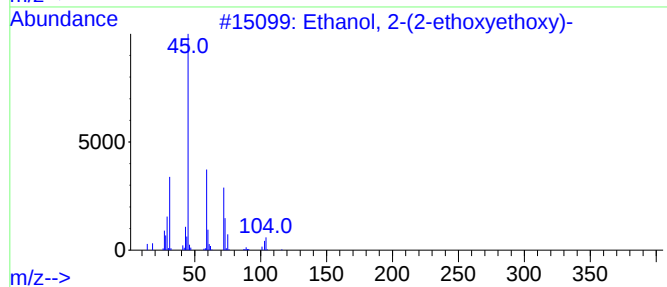
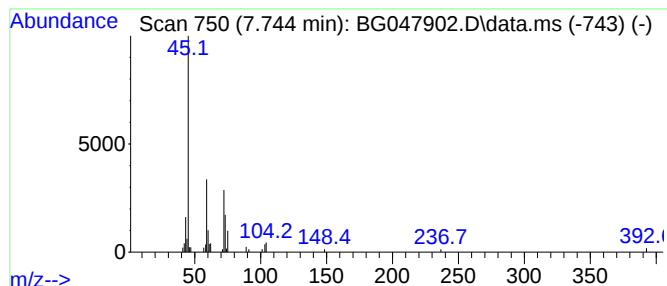
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Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.744	3.47 ng	51732	1,4-Dichlorobenzene-d4	8.161

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Diethyl carbitol	162	C8H18O3	000112-36-7	50
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	45
4			Ethyl 2-(2-(2-ethoxyethoxy)ethox...	220	C10H20O5	1000366-77-8	45
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45



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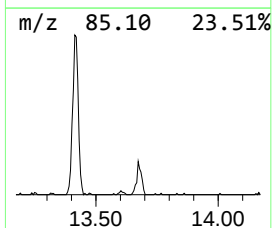
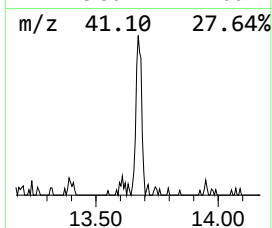
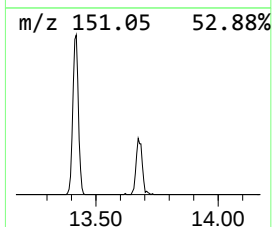
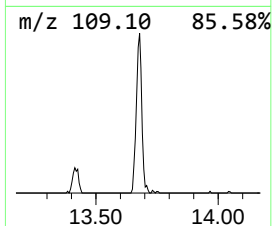
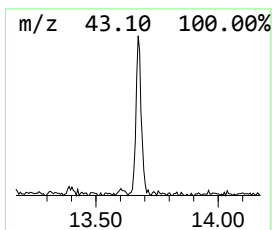
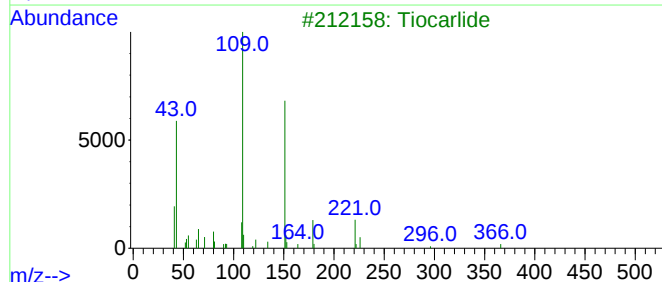
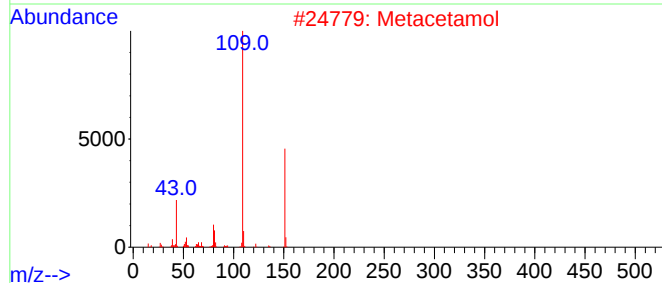
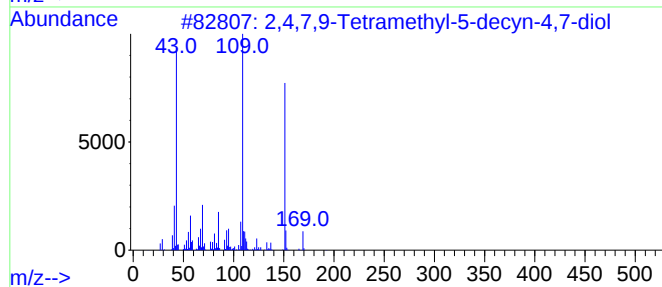
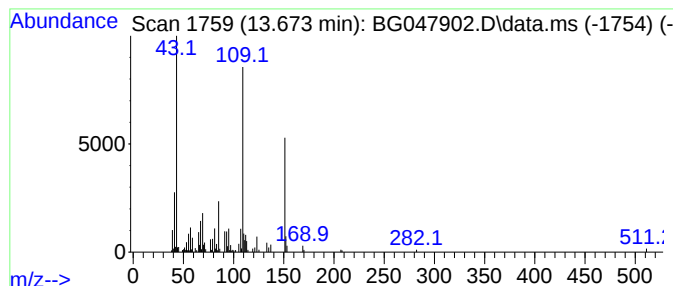
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.672	5.83 ng	173259	Acenaphthene-d10	14.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87		
2	Metacetamol	151	C8H9NO2	000621-42-1	58		
3	Tiocarlide	400	C23H32N2O2S	000910-86-1	53		
4	4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	53		
5	Acetaminophen	151	C8H9NO2	000103-90-2	53		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	3.508	4.6	ng	67985	1	8.161	298256	20.0
Propanoic acid,...	4.707	8.5	ng	126461	1	8.161	298256	20.0
Butanoic acid, ...	5.177	5.7	ng	84208	1	8.161	298256	20.0
Ethanol, 2-(2-e...	7.744	3.5	ng	51732	1	8.161	298256	20.0
2,4,7,9-Tetrame...	13.672	5.8	ng	173259	3	14.789	593983	20.0