

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
 Data File : BG060194.D
 Acq On : 2 Jan 2024 14:29
 Operator : MA/JU
 Sample : 06027-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CURB

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: BG060194.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.118	3	5	10	rVB	355377	366205	2.02%	0.502%
2	4.445	225	231	240	rBV	195285	311895	1.72%	0.428%
3	5.039	326	332	342	rBV	1583398	2294901	12.67%	3.147%
4	5.509	406	412	427	rBV	2815766	4413604	24.36%	6.052%
5	7.101	674	683	702	rBV	3118153	5477819	30.24%	7.512%
6	7.941	817	826	834	rBV	559429	1005798	5.55%	1.379%
7	9.099	1015	1023	1038	rBV	1918742	3403553	18.79%	4.667%
8	10.744	1294	1303	1315	rBV	847833	1548851	8.55%	2.124%
9	13.200	1711	1721	1732	rBV	6545879	10344073	57.10%	14.185%
10	14.575	1949	1955	1963	rBV	1844782	2806315	15.49%	3.848%
11	16.061	2201	2208	2221	rBV	3872368	5811855	32.08%	7.970%
12	17.324	2416	2423	2434	rBV	2687418	4154572	22.93%	5.697%
13	19.945	2863	2869	2878	rBV	13133970	18116614	100.00%	24.844%
14	20.245	2917	2920	2924	rVB	159327	186741	1.03%	0.256%
15	20.738	3000	3004	3008	rBV2	211010	257588	1.42%	0.353%
16	21.238	3084	3089	3101	rBV2	698504	1090517	6.02%	1.495%
17	21.590	3142	3149	3163	rBV2	2647315	4475099	24.70%	6.137%
18	21.778	3177	3181	3187	rVB	237753	342066	1.89%	0.469%
19	22.383	3279	3284	3290	rVB2	218943	341592	1.89%	0.468%
20	23.065	3395	3400	3406	rVB3	177316	338451	1.87%	0.464%
21	23.858	3530	3535	3543	rVB5	125046	267960	1.48%	0.367%
22	24.228	3592	3598	3606	rVB4	104628	240165	1.33%	0.329%
23	24.763	3679	3689	3712	rVB2	1645556	4846272	26.75%	6.646%
24	25.491	3807	3813	3825	rVB8	87653	282589	1.56%	0.388%
25	27.072	4074	4082	4092	rBV9	60232	197783	1.09%	0.271%

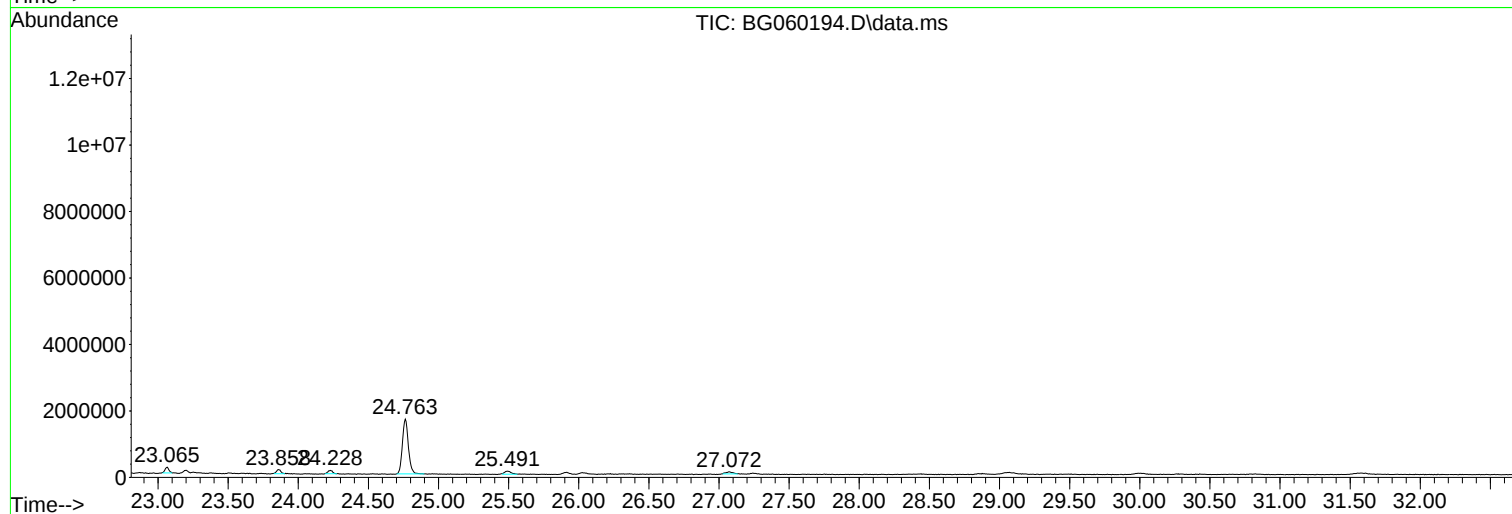
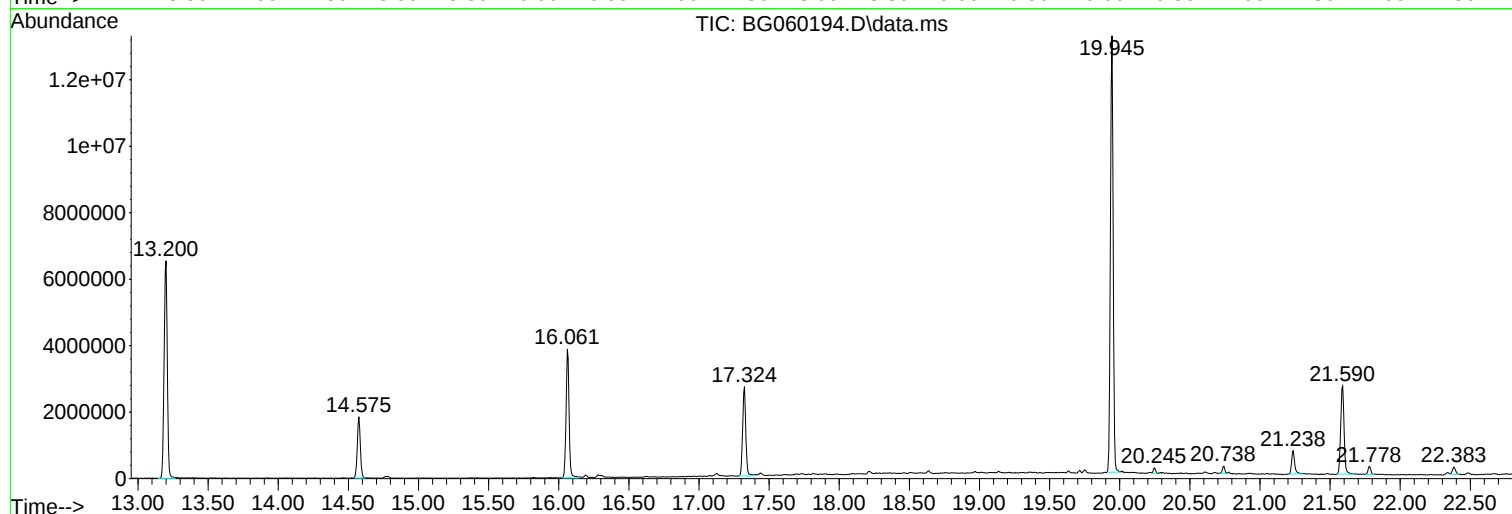
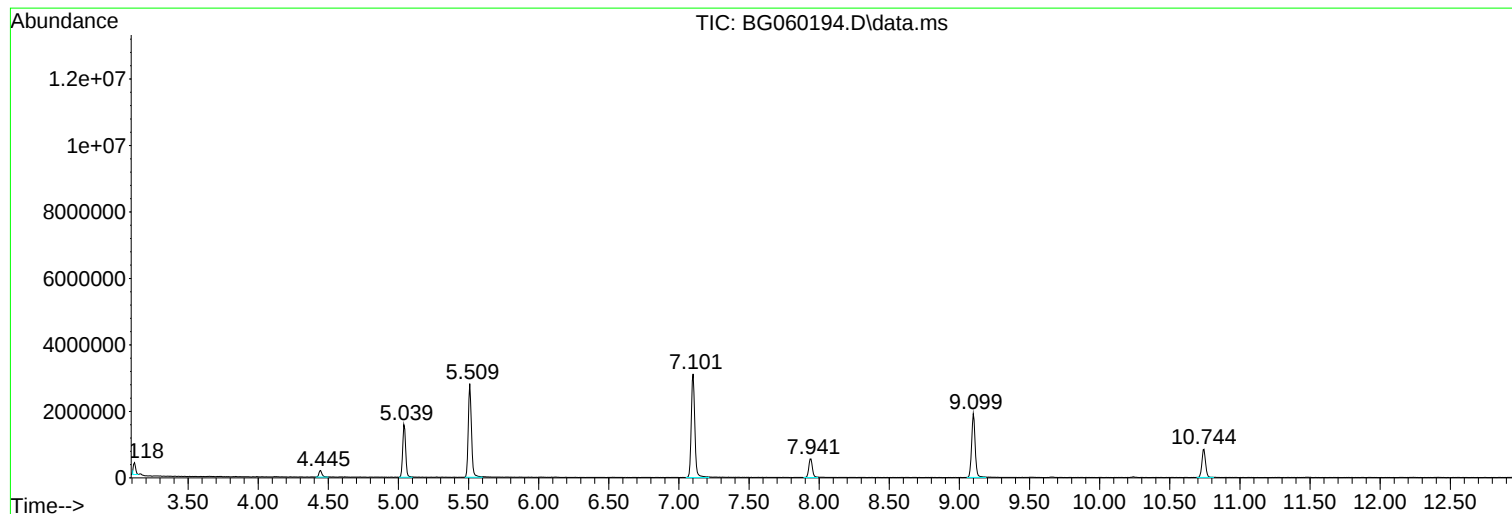
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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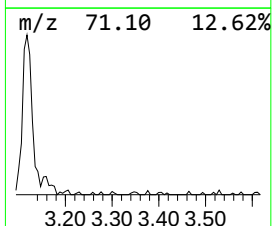
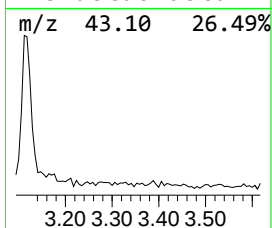
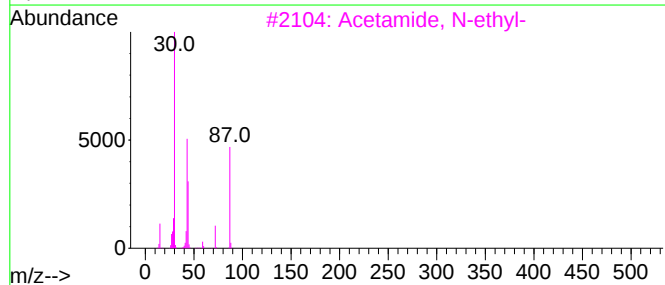
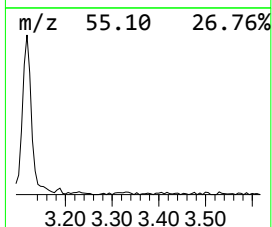
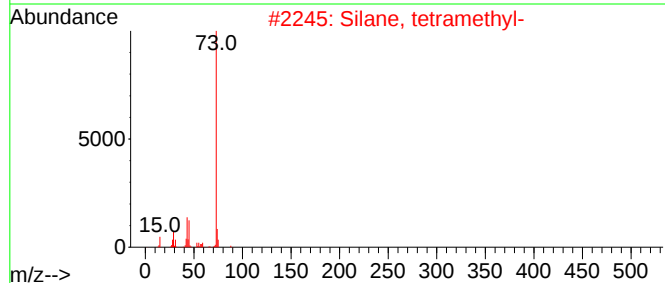
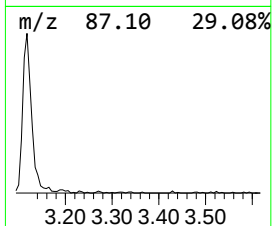
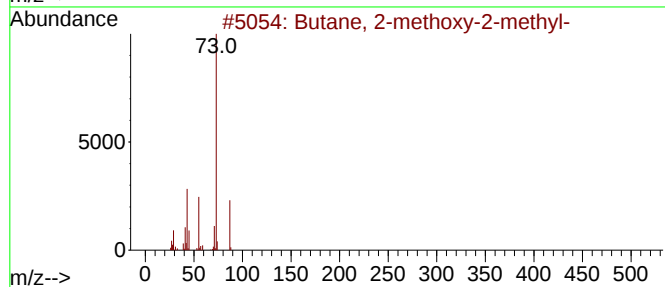
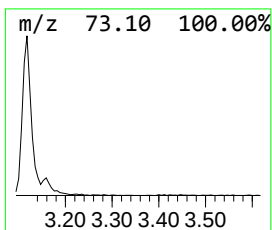
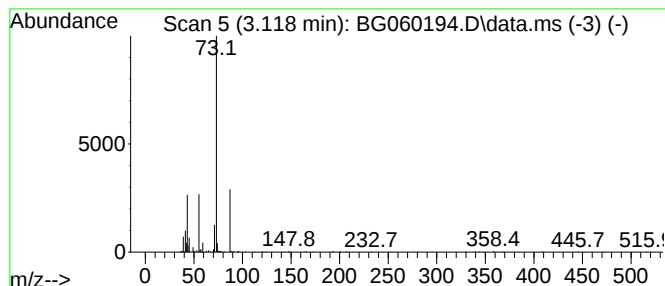
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.118	7.28 ng	366205	1,4-Dichlorobenzene-d4	7.941

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9



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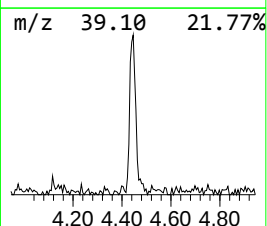
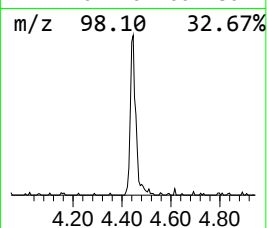
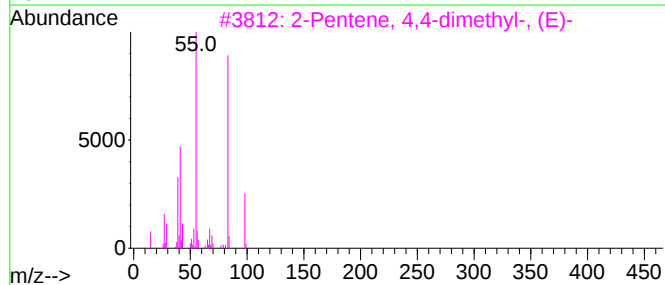
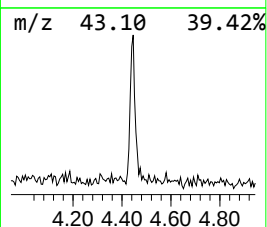
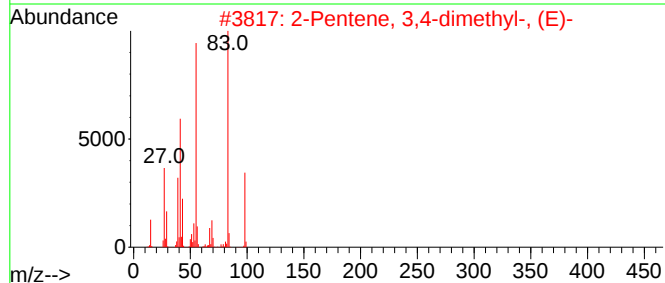
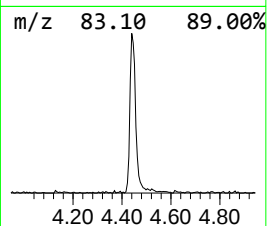
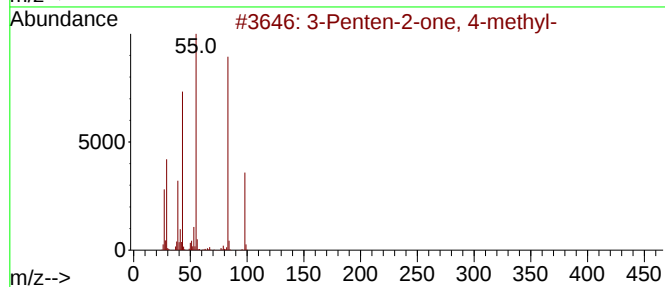
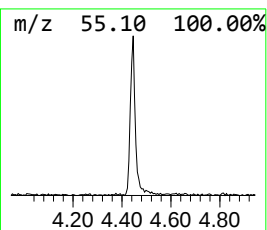
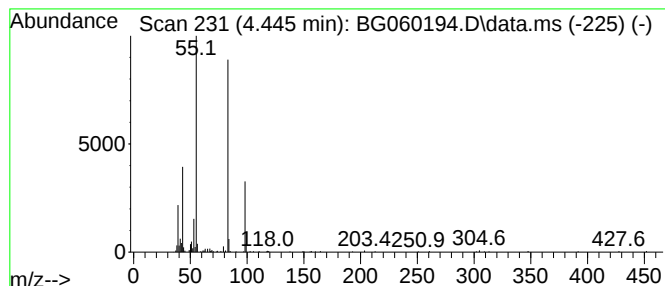
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.445	6.20 ng	311895	1,4-Dichlorobenzene-d4	7.941

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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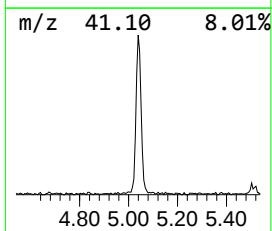
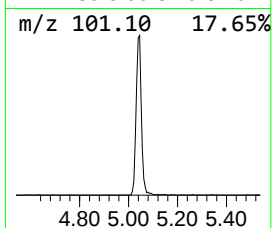
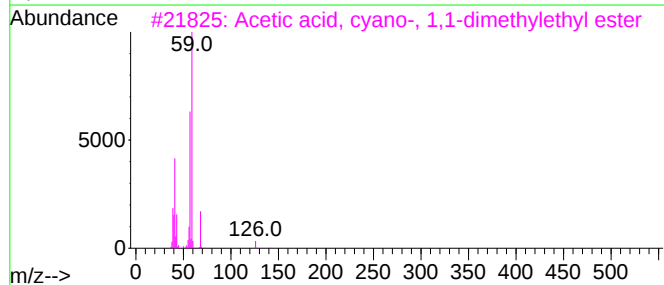
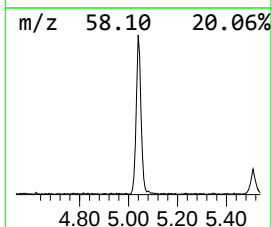
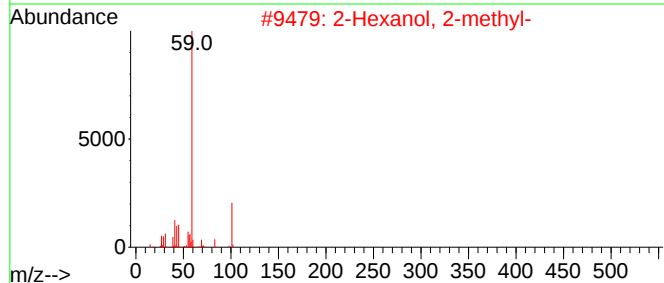
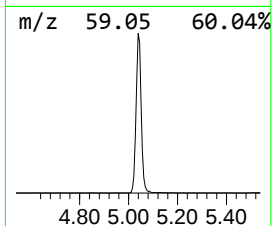
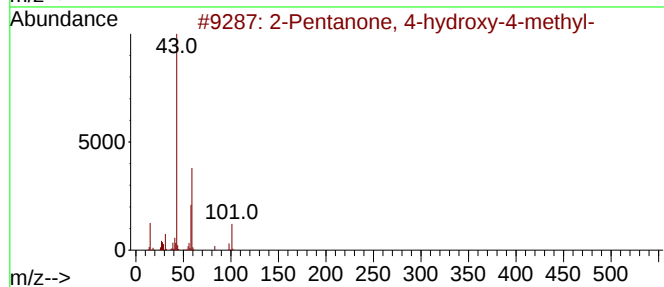
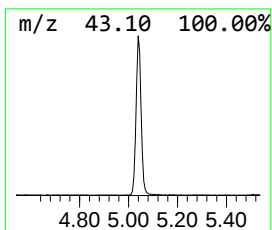
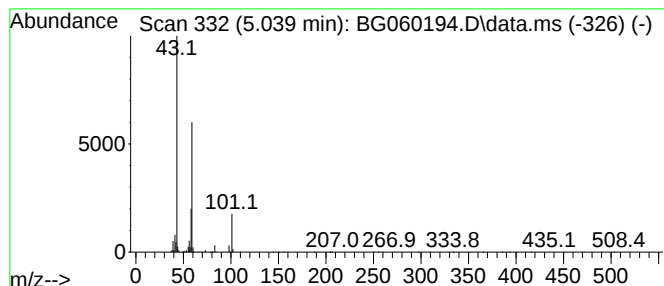
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.039	45.63 ng	2294900	1,4-Dichlorobenzene-d4			7.941
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	37
3	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	32
4	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	28
5	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	25



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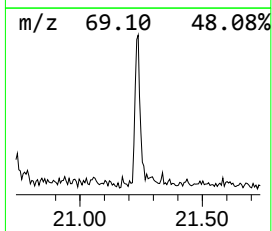
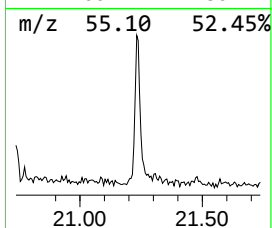
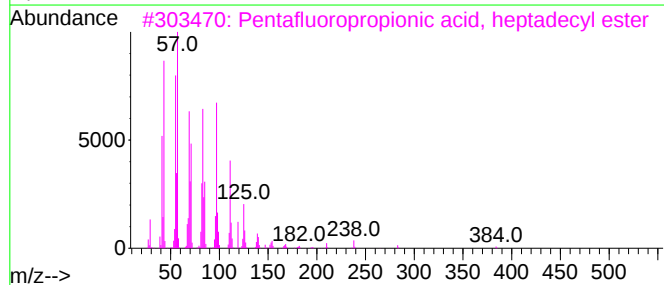
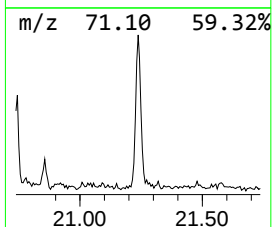
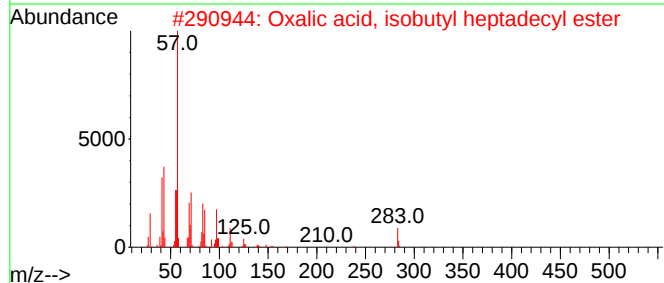
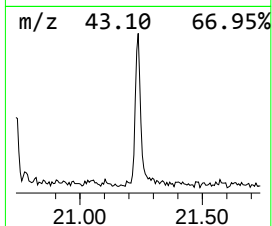
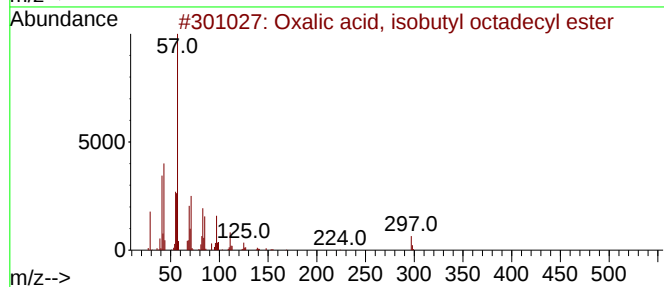
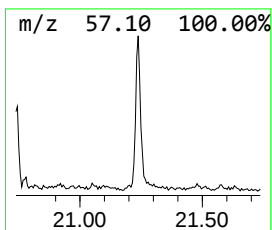
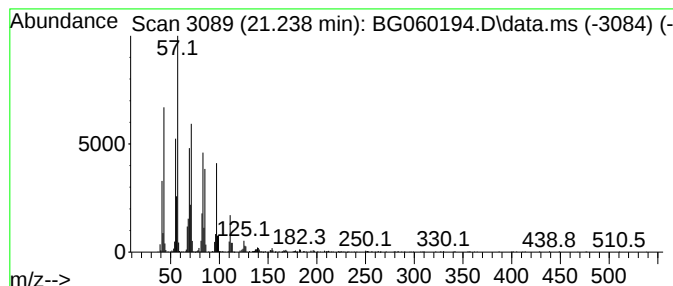
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Peak Number 4 Oxalic acid, isobutyl octadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.238	4.87 ng	1090520	Chrysene-d12	21.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	74
2			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	74
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	68
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	68
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	68



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.118	7.3	ng	366205	1	7.941	1005800	20.0
3-Penten-2-one,...	4.445	6.2	ng	311895	1	7.941	1005800	20.0
2-Pentanone, 4-...	5.039	45.6	ng	2294900	1	7.941	1005800	20.0
Oxalic acid, is...	21.238	4.9	ng	1090520	5	21.590	4475100	20.0