

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
 Data File : BG055556.D
 Acq On : 11 Nov 2022 2:28
 Operator : CG/JU
 Sample : N5494-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-18

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055556.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.329	3	7	22	rVB	278897	520898	17.54%	3.568%
2	4.709	237	242	248	rBV	40538	58782	1.98%	0.403%
3	5.326	339	347	357	rBV	323723	506717	17.07%	3.471%
4	5.796	419	427	438	rBV	766187	1220366	41.10%	8.359%
5	7.400	692	700	709	rBV	792757	1343938	45.26%	9.205%
6	8.270	841	848	854	rBV	157138	268093	9.03%	1.836%
7	9.439	1039	1047	1057	rBV	444822	800999	26.98%	5.487%
8	11.096	1321	1329	1337	rVB	220104	390098	13.14%	2.672%
9	13.511	1733	1740	1749	rBV	1198558	1911863	64.39%	13.095%
10	14.886	1966	1974	1982	rBV	354644	553363	18.64%	3.790%
11	16.360	2218	2225	2239	rBV	929417	1417666	47.75%	9.710%
12	17.624	2433	2440	2446	rBV	463337	700975	23.61%	4.801%
13	18.487	2582	2587	2603	rBV	57653	94376	3.18%	0.646%
14	19.745	2797	2801	2811	rBV6	22619	36282	1.22%	0.249%
15	20.215	2875	2881	2889	rVB	2256511	2969126	100.00%	20.337%
16	21.531	3100	3105	3111	rBV3	101980	157566	5.31%	1.079%
17	21.789	3146	3149	3155	rVB2	20141	30113	1.01%	0.206%
18	21.919	3165	3171	3178	rBV2	472850	795654	26.80%	5.450%
19	23.711	3473	3476	3485	rVB5	24172	44732	1.51%	0.306%
20	25.338	3743	3753	3765	rBV	267646	777806	26.20%	5.328%

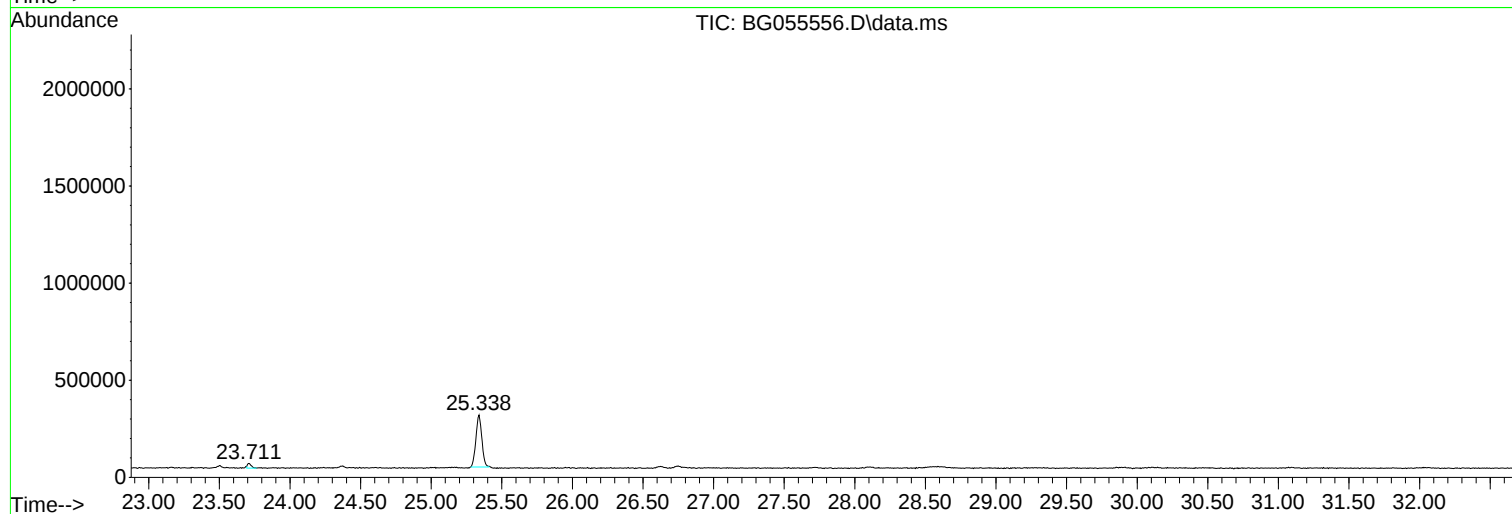
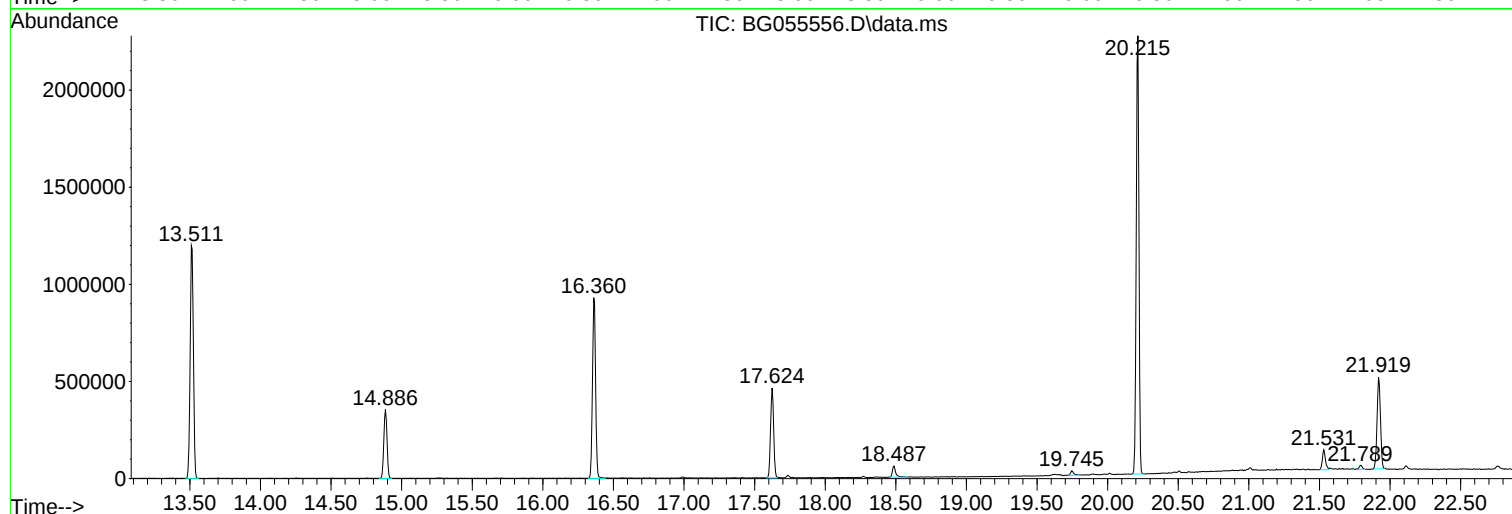
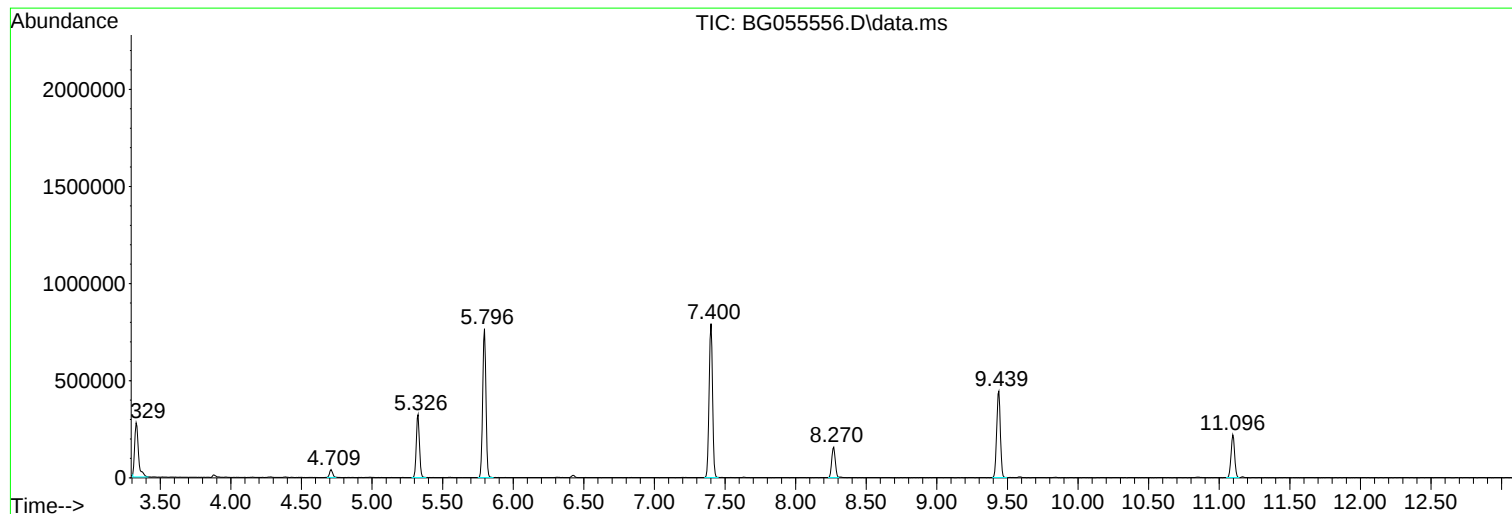
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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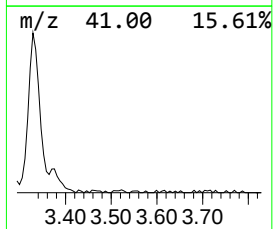
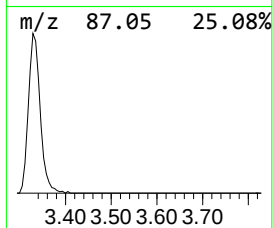
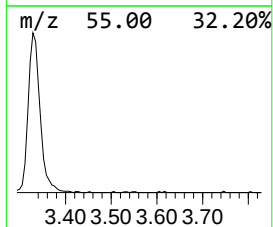
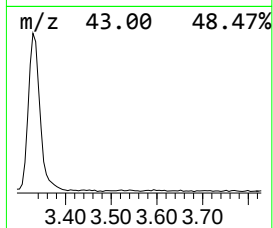
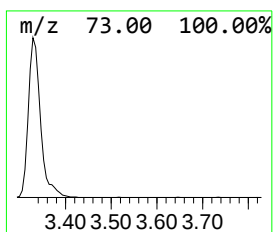
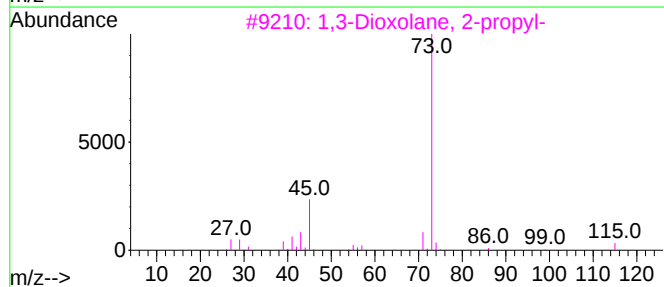
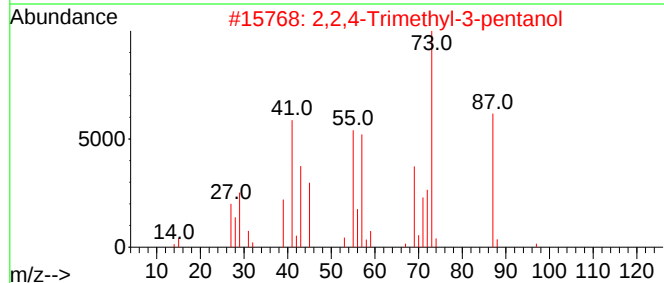
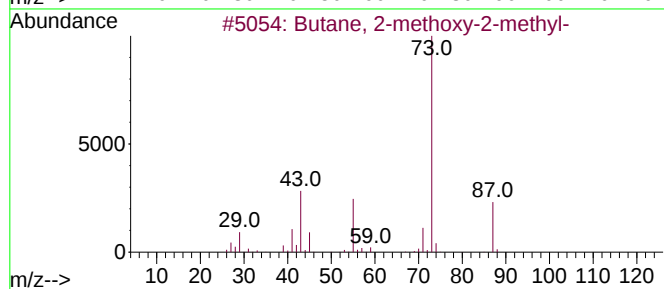
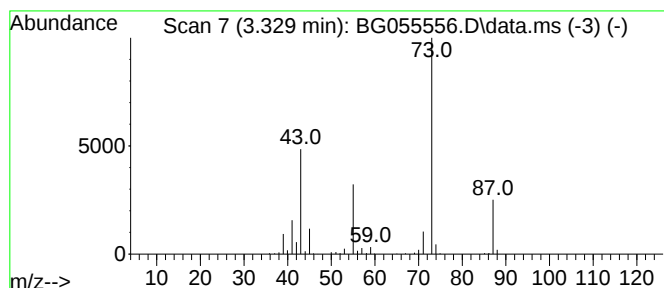
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.329	38.86 ng	520898	1,4-Dichlorobenzene-d4	8.270

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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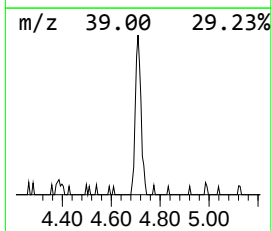
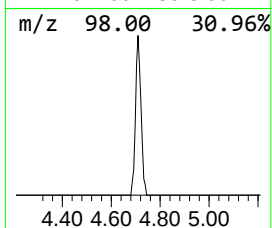
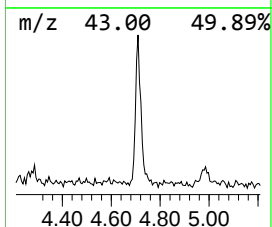
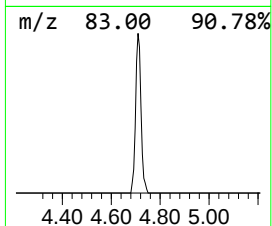
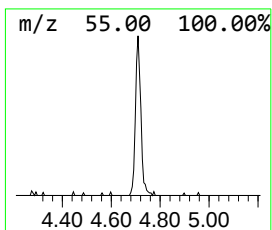
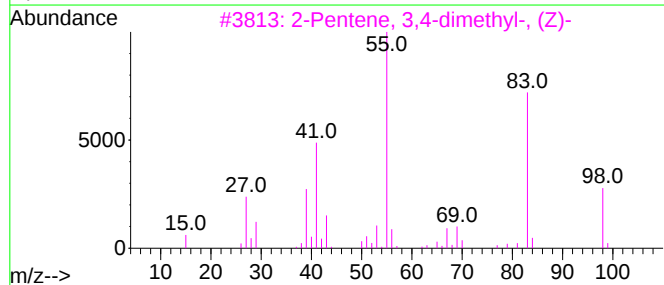
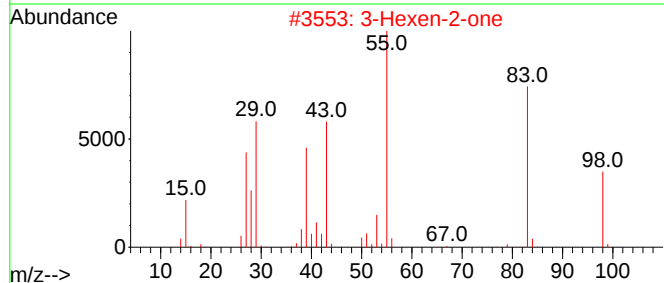
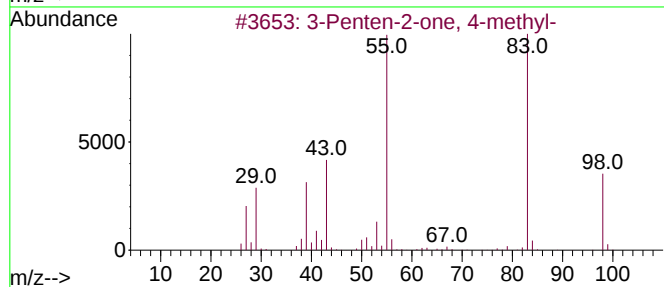
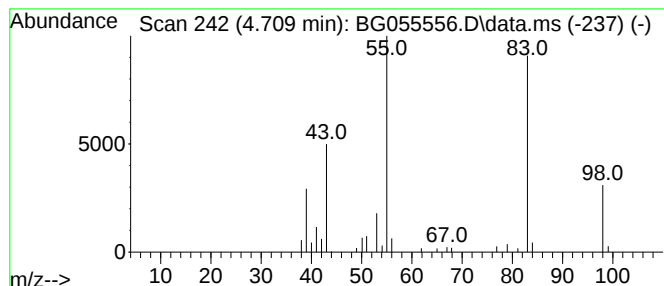
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.709	4.39 ng	58782	1,4-Dichlorobenzene-d4	8.270

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72



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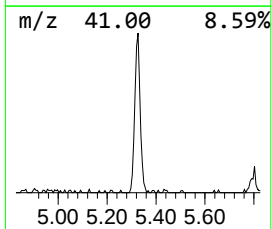
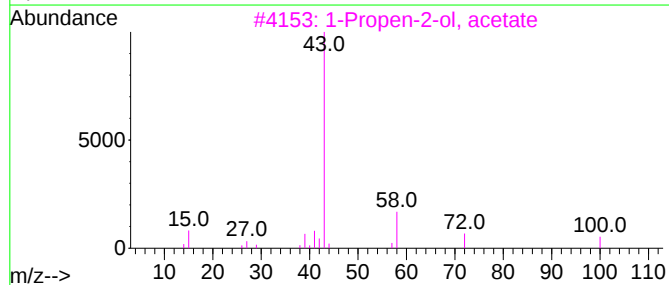
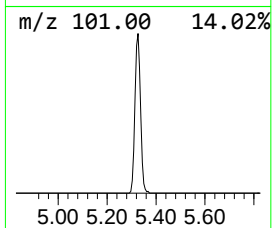
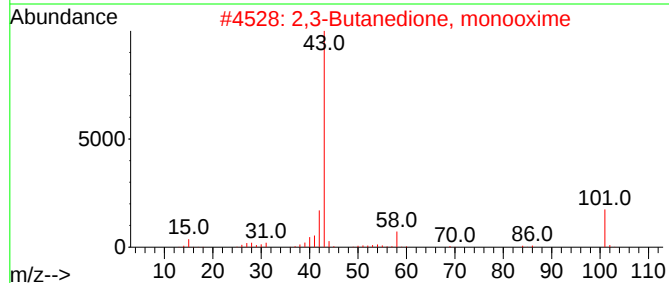
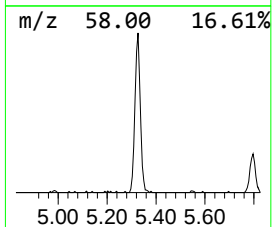
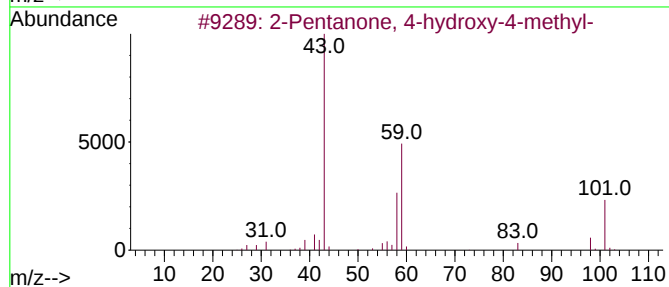
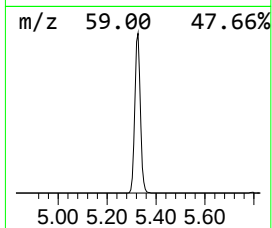
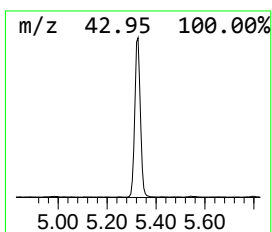
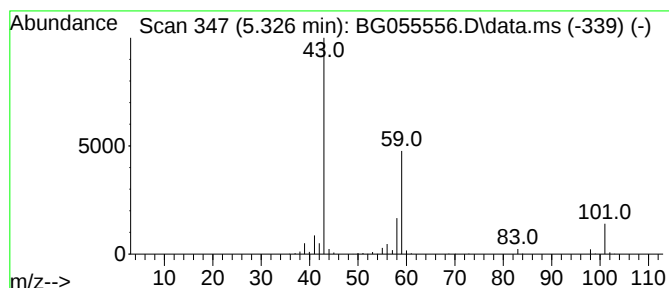
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.326	37.80 ng	506717	1,4-Dichlorobenzene-d4	8.270

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5			5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9



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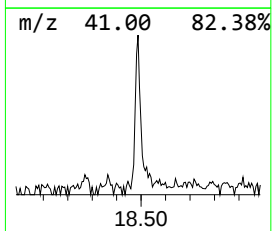
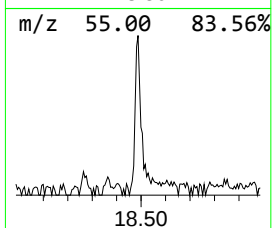
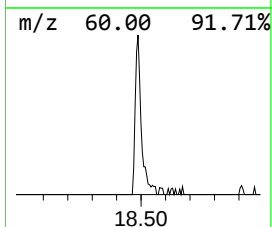
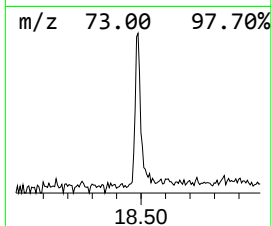
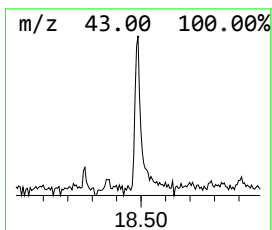
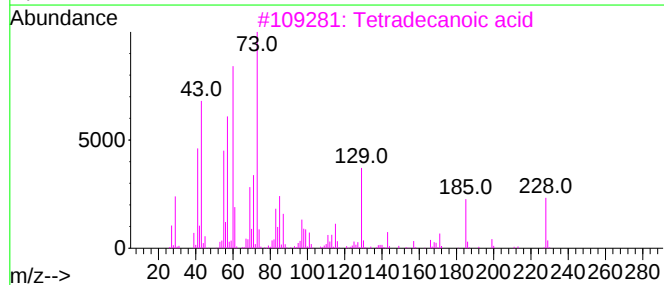
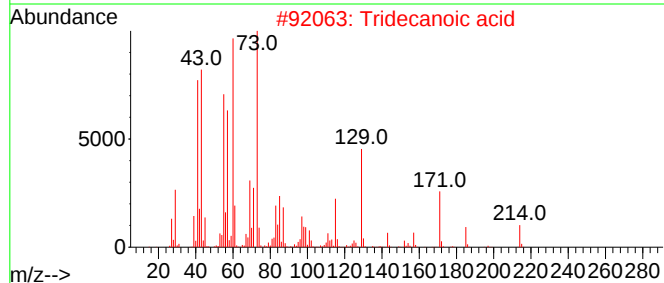
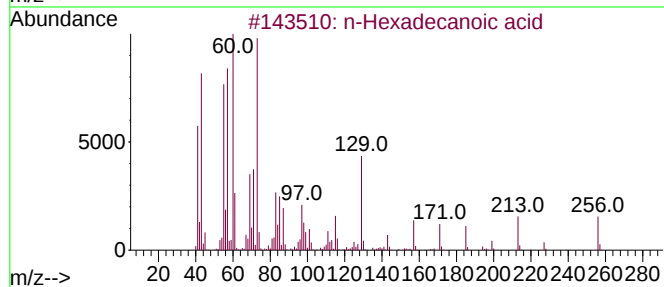
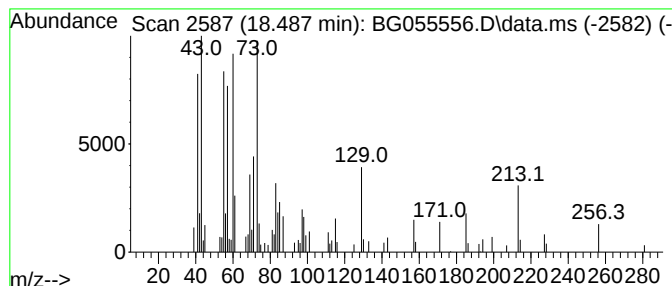
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.487	2.69 ng	94376	Phenanthrene-d10	17.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	76
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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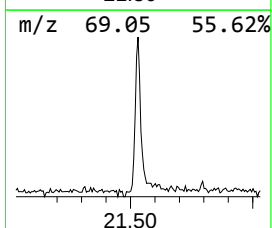
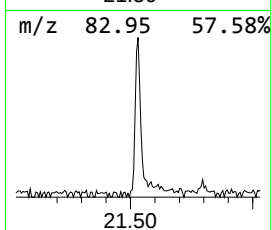
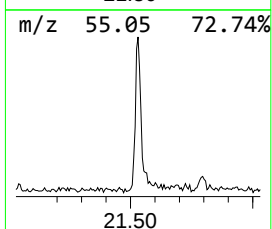
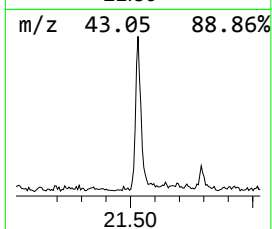
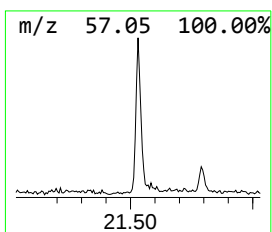
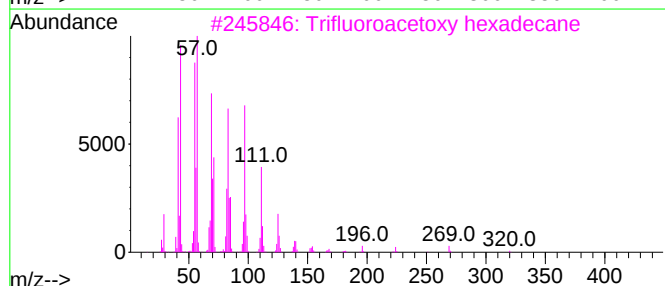
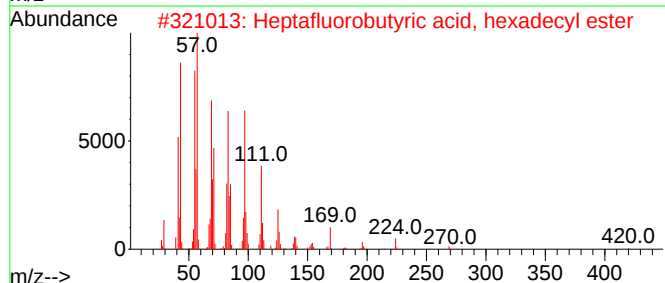
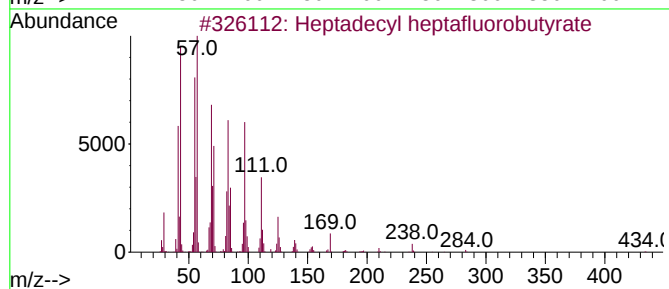
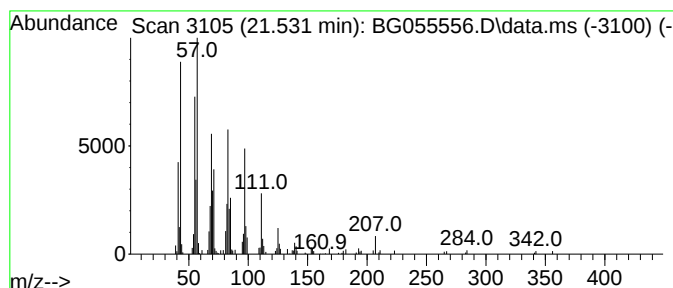
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.531	3.96 ng	157566	Chrysene-d12	21.919	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.329	38.9	ng	520898	1	8.270	268093	20.0
3-Penten-2-one,...	4.709	4.4	ng	58782	1	8.270	268093	20.0
2-Pentanone, 4-...	5.326	37.8	ng	506717	1	8.270	268093	20.0
n-Hexadecanoic ...	18.487	2.7	ng	94376	4	17.624	700975	20.0
Heptadecyl hept...	21.531	4.0	ng	157566	5	21.919	795654	20.0