

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071524\
 Data File : BF138567.D
 Acq On : 15 Jul 2024 13:57
 Operator : CG\JU
 Sample : PB162036BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB162036BL

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_F\Methods\8270-BF070924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138567.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	23	29	34	rVB	100788	130529	2.07%	0.365%
2	5.122	511	516	527	rVB	226157	358661	5.70%	1.004%
3	5.510	576	582	585	rBV	4342012	4383493	69.61%	12.270%
4	6.504	745	751	754	rBV	3996177	4968539	78.90%	13.907%
5	6.863	809	812	816	rBV	1103392	934944	14.85%	2.617%
6	7.433	902	909	912	rBV	2607184	2914461	46.28%	8.158%
7	8.145	1025	1030	1034	rBV	1303433	1211753	19.24%	3.392%
8	9.227	1207	1214	1217	rBV	4883185	5047379	80.15%	14.128%
9	9.898	1322	1328	1332	rBV	1529964	1431039	22.72%	4.006%
10	10.692	1457	1463	1467	rBV	3500619	3711654	58.94%	10.389%
11	11.386	1577	1581	1585	rBV	1927572	1647360	26.16%	4.611%
12	12.633	1788	1793	1796	rBV	116930	86036	1.37%	0.241%
13	12.786	1816	1819	1822	rVB	348762	264769	4.20%	0.741%
14	12.974	1846	1851	1854	rBV	5623956	6297652	100.00%	17.627%
15	13.492	1933	1939	1942	rBV	209789	177591	2.82%	0.497%
16	13.757	1979	1984	1997	rVB7	19608	65649	1.04%	0.184%
17	14.021	2025	2029	2038	rBV	1322706	1292032	20.52%	3.616%
18	15.492	2274	2279	2293	rBV	559451	803109	12.75%	2.248%

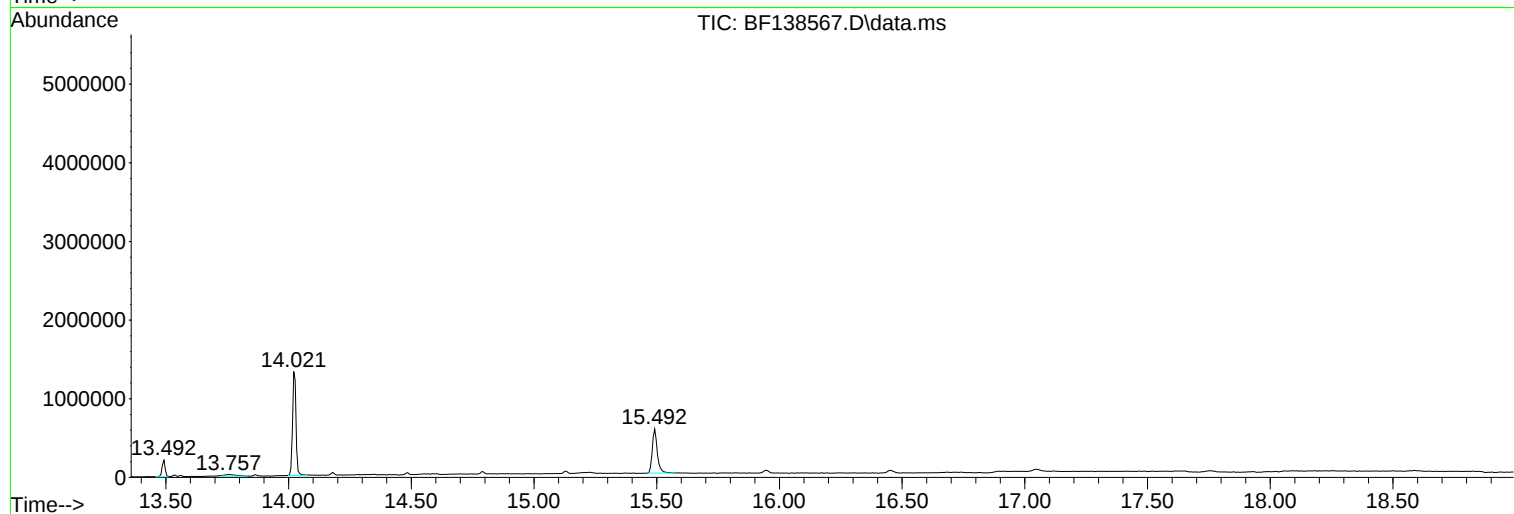
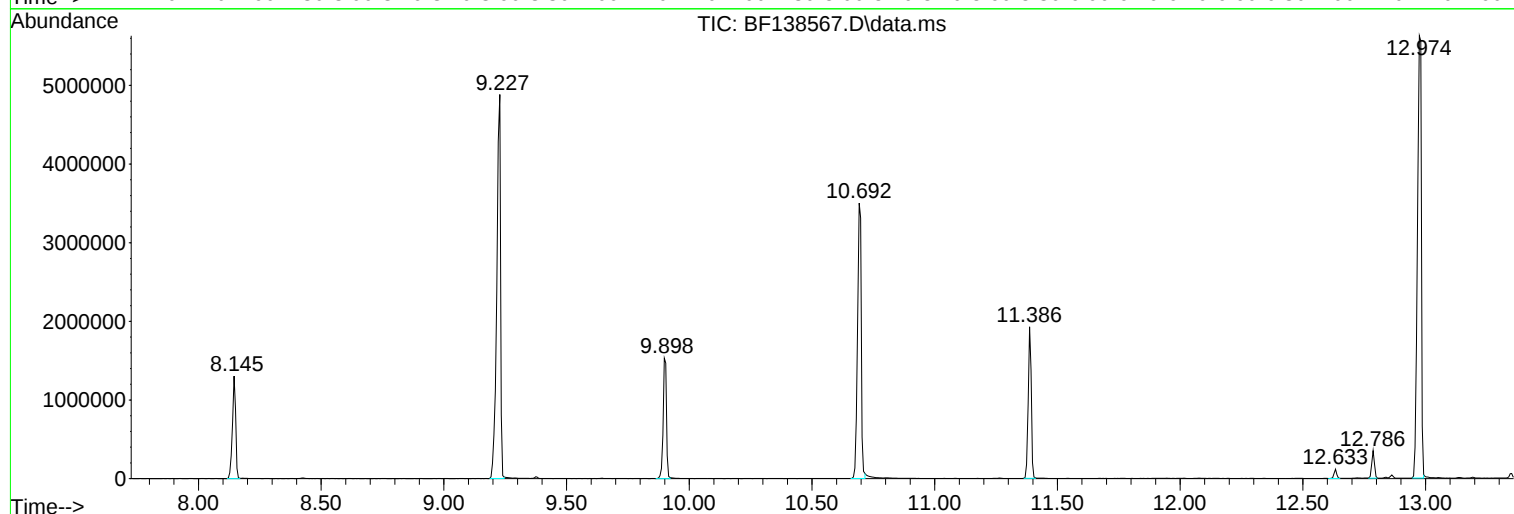
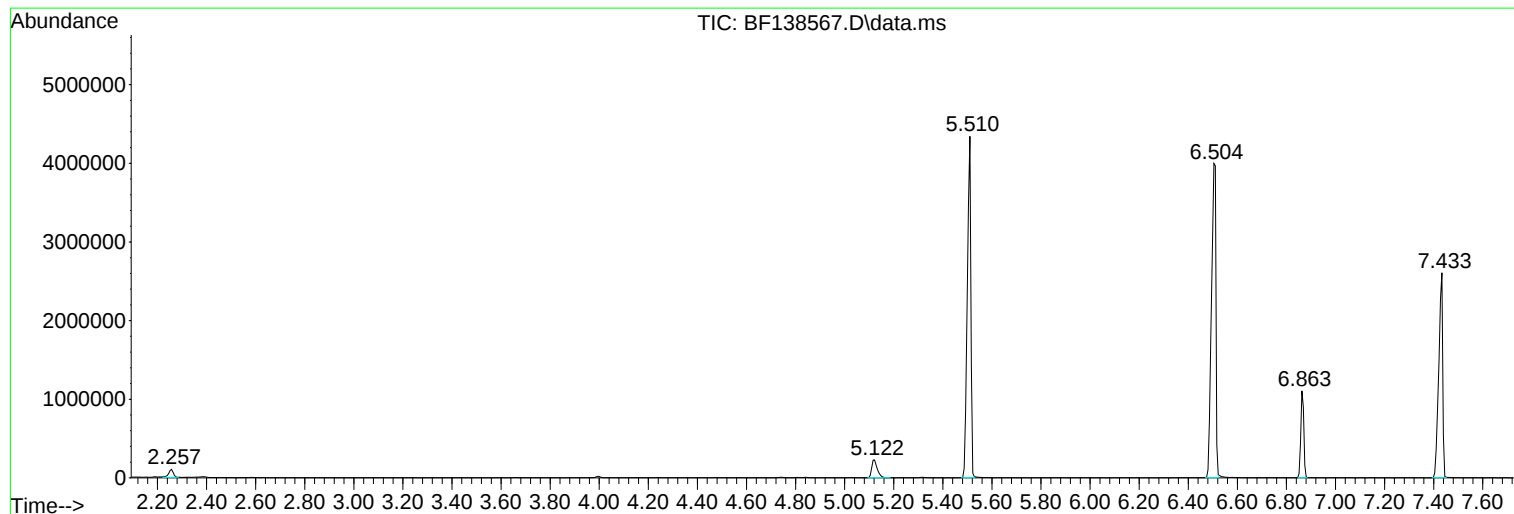
Sum of corrected areas: 35726650

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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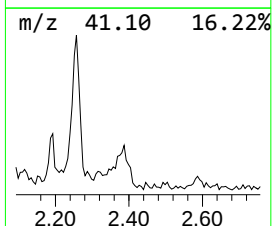
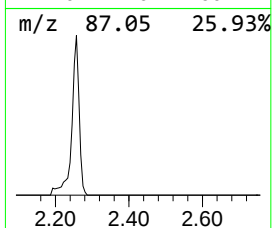
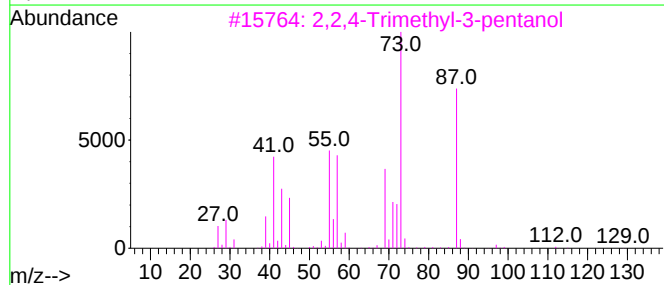
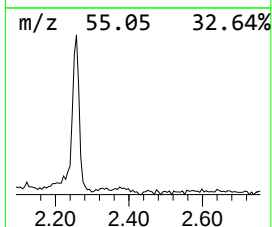
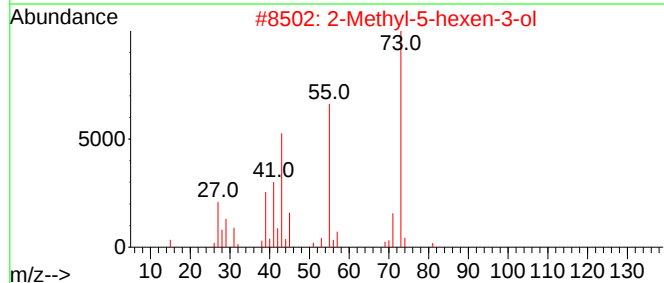
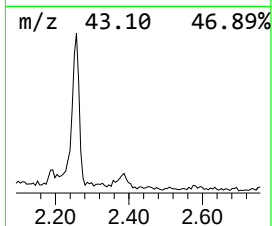
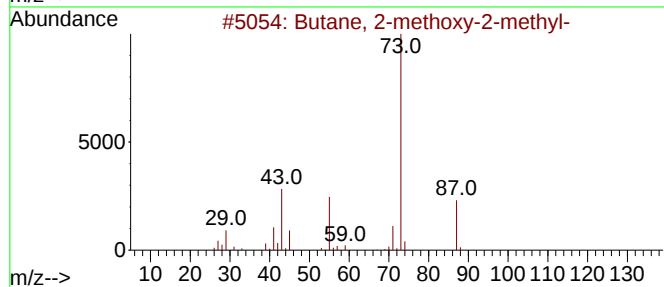
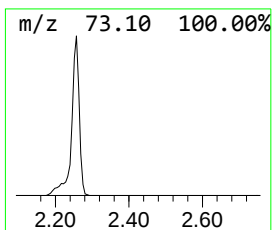
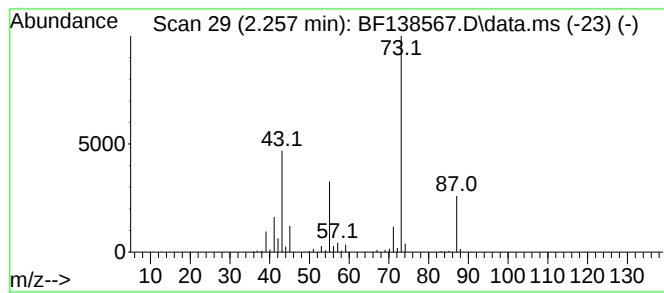
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	2.79 ng	130529	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	50
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	23



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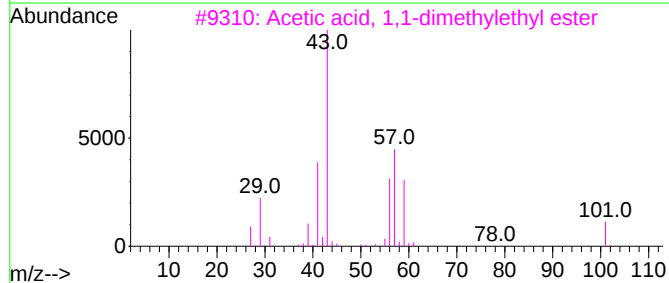
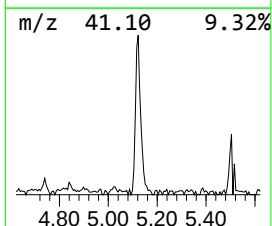
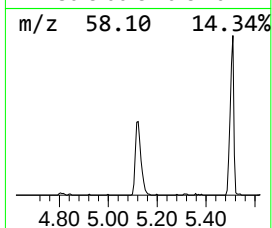
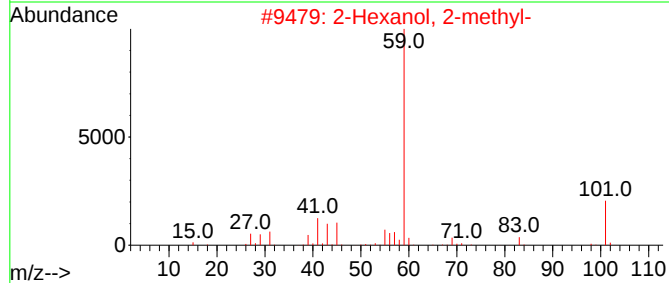
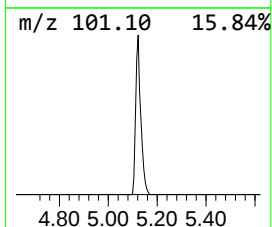
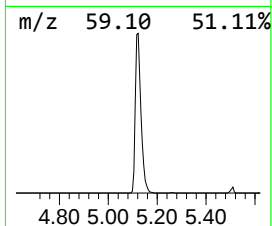
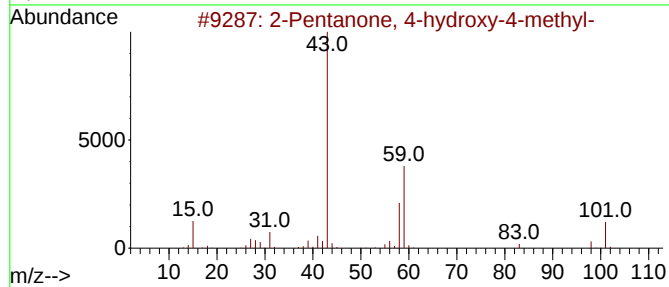
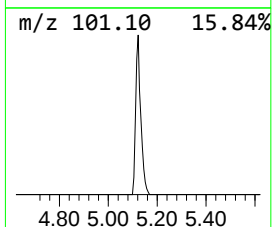
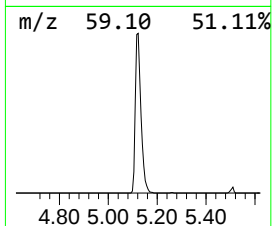
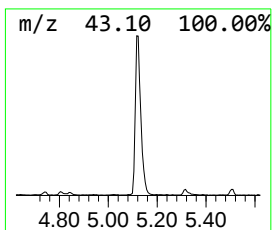
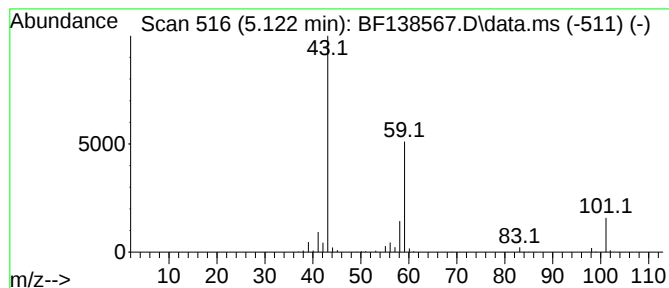
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.122	7.67 ng	358661	1,4-Dichlorobenzene-d4	6.863	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9



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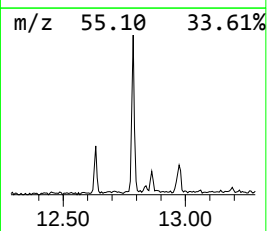
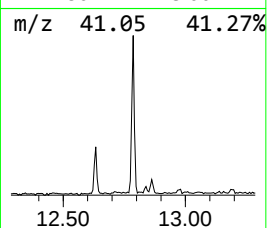
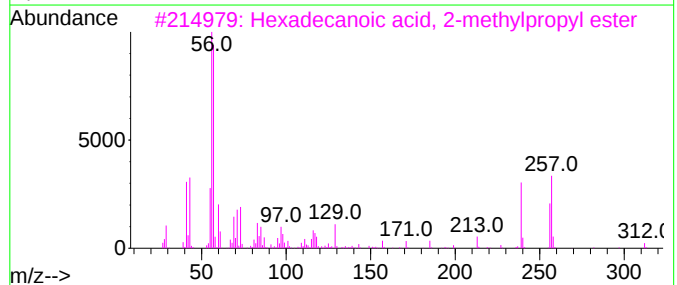
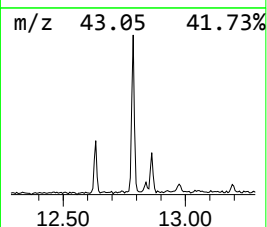
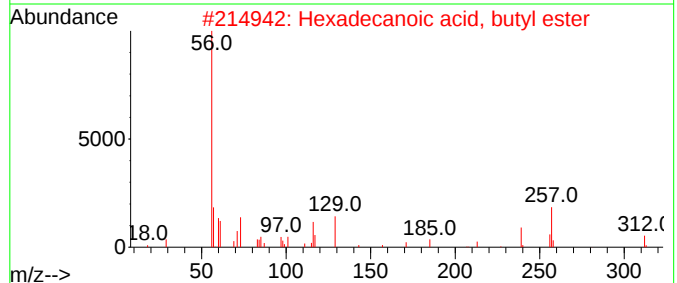
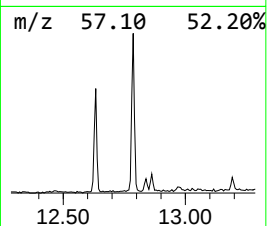
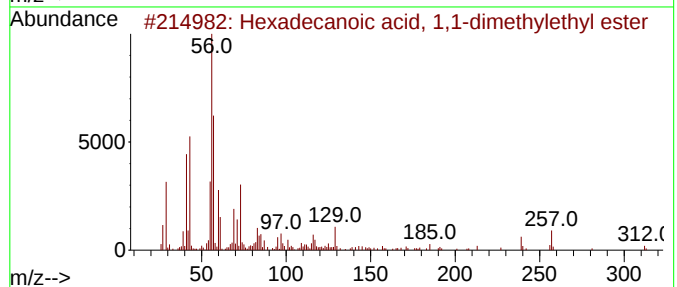
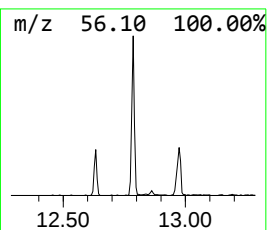
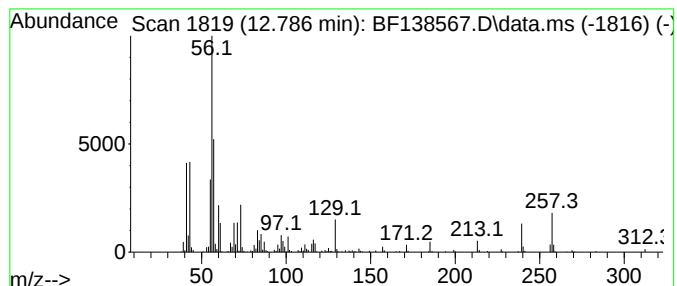
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Peak Number 3 Hexadecanoic acid, 1,1-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	4.10 ng	264769	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	92
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	72
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	60
4			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	47
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38



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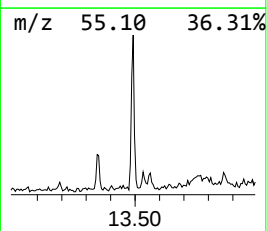
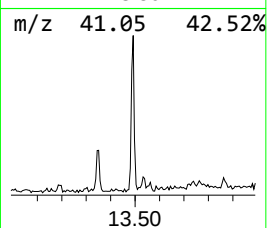
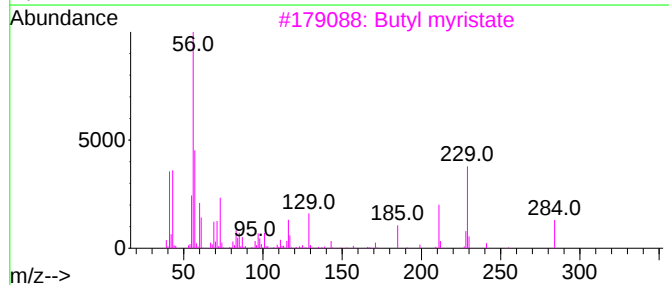
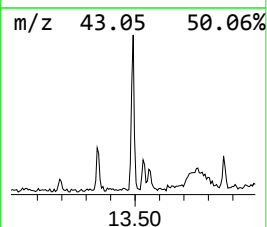
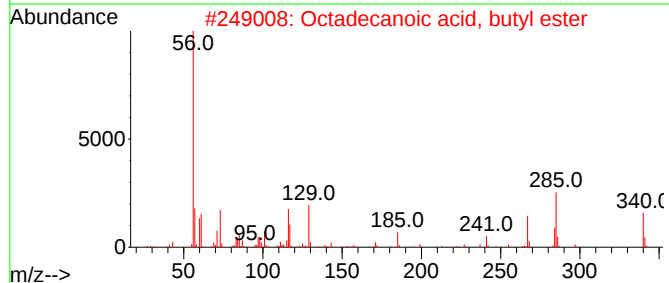
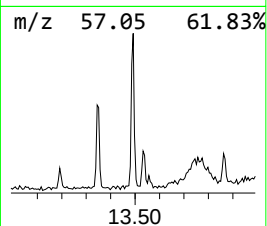
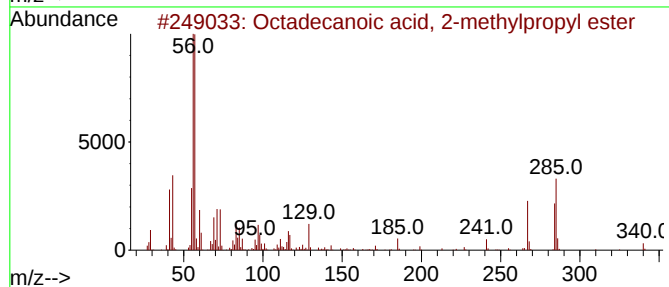
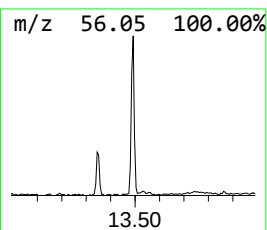
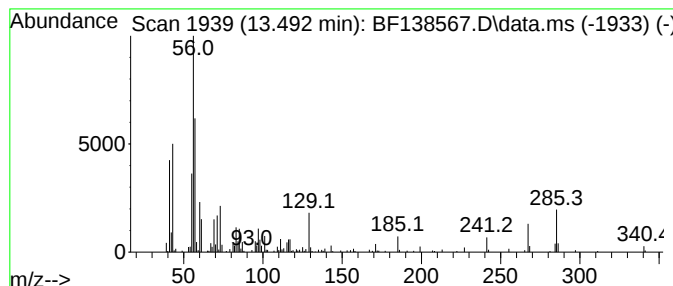
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid, 2-methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	2.75 ng	177591	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	90
2			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	78
3			Butyl myristate	284	C18H36O2	000110-36-1	64
4			Docosanoic acid	340	C22H44O2	000112-85-6	42
5			Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.257	2.8	ng	130529	1	6.863	934944	20.0
2-Pentanone, 4-...	5.122	7.7	ng	358661	1	6.863	934944	20.0
Hexadecanoic ac...	12.786	4.1	ng	264769	5	14.021	1292030	20.0
Octadecanoic ac...	13.492	2.8	ng	177591	5	14.021	1292030	20.0