

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071524\
 Data File : BF138565.D
 Acq On : 15 Jul 2024 12:52
 Operator : CG\JU
 Sample : PB162035BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB162035BL

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: BF138565.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	21	29	37	rVB	101155	150611	2.93%	0.447%
2	5.122	511	516	526	rVB	255521	395930	7.69%	1.174%
3	5.510	577	582	585	rBV	4799990	4801323	93.26%	14.237%
4	6.510	746	752	755	rBV	3865106	4452803	86.49%	13.204%
5	6.863	809	812	816	rBV	1086282	984819	19.13%	2.920%
6	7.433	902	909	912	rBV	2658152	2907862	56.48%	8.623%
7	8.145	1025	1030	1034	rBV	1322426	1215090	23.60%	3.603%
8	9.227	1207	1214	1217	rBV	5135331	5032739	97.75%	14.924%
9	9.904	1323	1329	1332	rBV	1587387	1398375	27.16%	4.147%
10	10.698	1456	1464	1467	rBV	2953107	3038651	59.02%	9.011%
11	11.386	1577	1581	1585	rBV	1656814	1456417	28.29%	4.319%
12	12.633	1790	1793	1797	rBV	98808	74795	1.45%	0.222%
13	12.786	1816	1819	1822	rBV	271221	208136	4.04%	0.617%
14	12.980	1846	1852	1854	rBV	4717788	5148437	100.00%	15.267%
15	13.492	1934	1939	1944	rBV	182753	156793	3.05%	0.465%
16	14.021	2025	2029	2039	rBV	1051632	1046809	20.33%	3.104%
17	14.792	2156	2160	2166	rBV	43586	52732	1.02%	0.156%
18	15.492	2274	2279	2290	rBV	753306	1064265	20.67%	3.156%
19	15.945	2352	2356	2362	rBV2	42762	73855	1.43%	0.219%
20	16.451	2439	2442	2449	rVB3	39597	62792	1.22%	0.186%

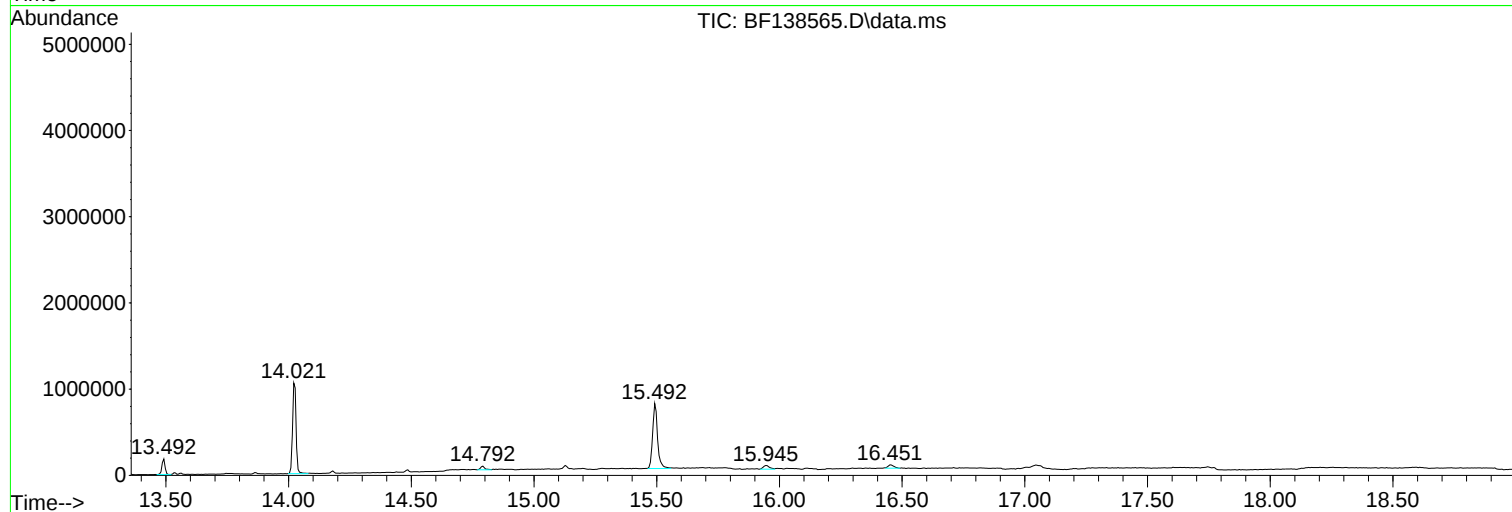
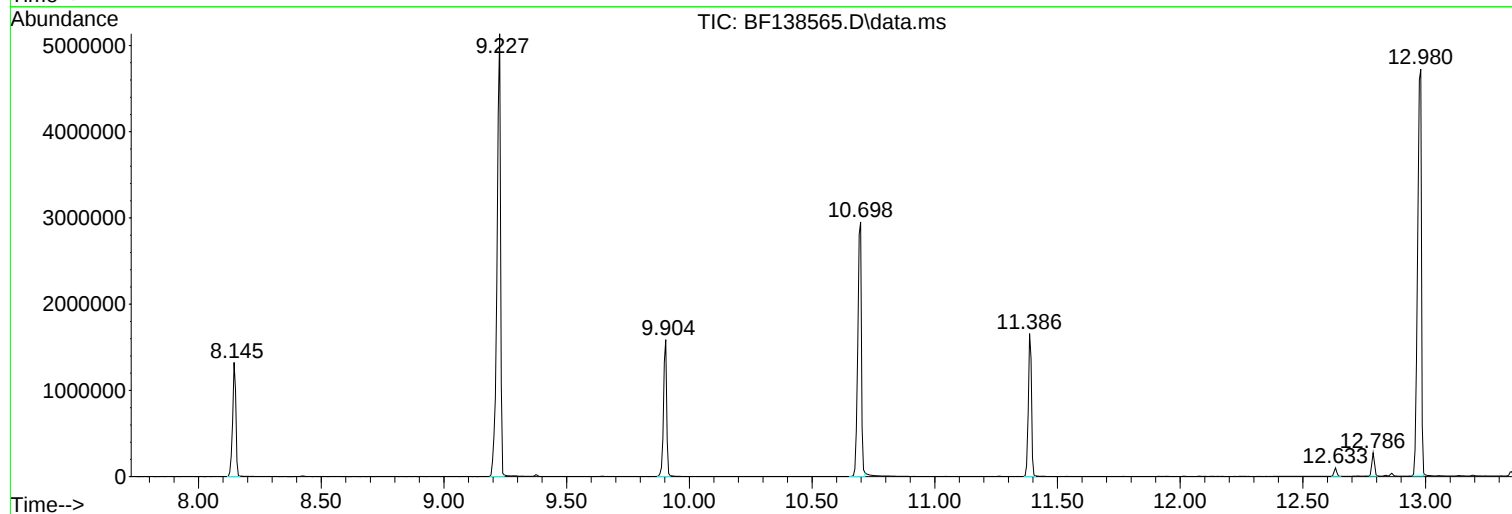
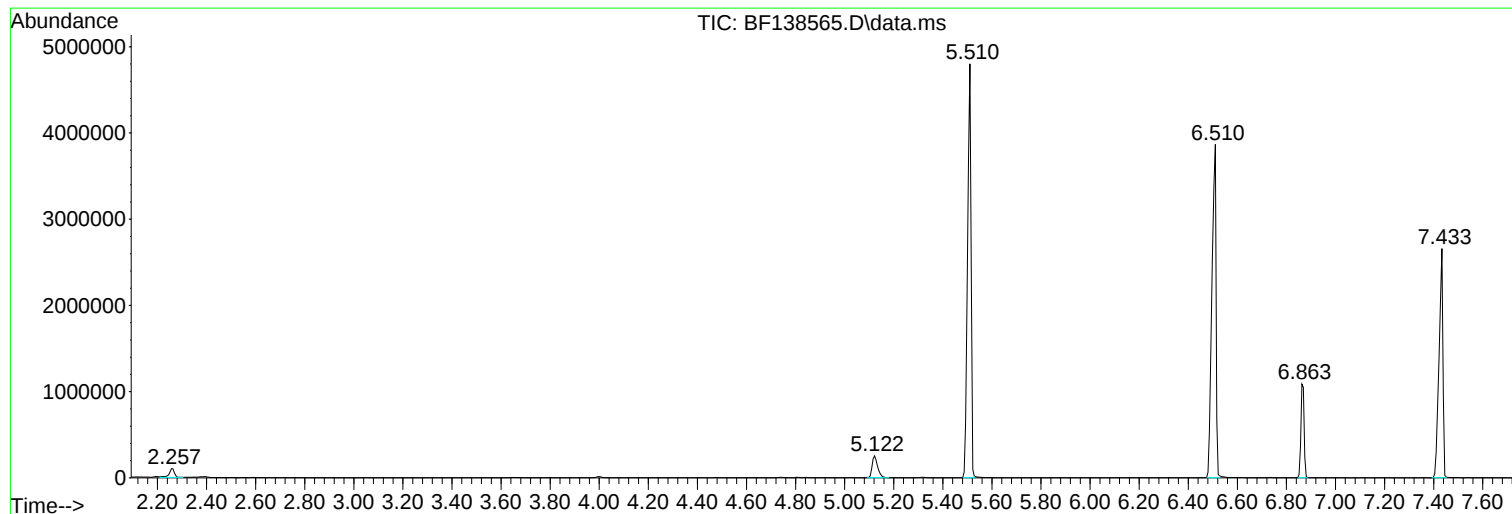
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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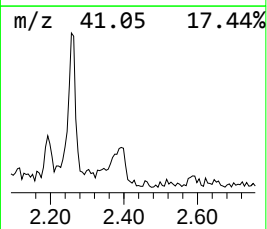
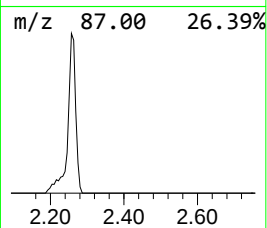
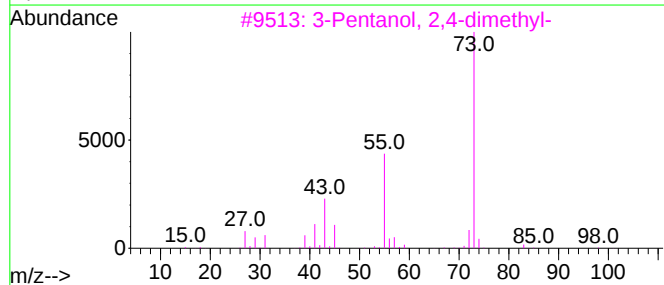
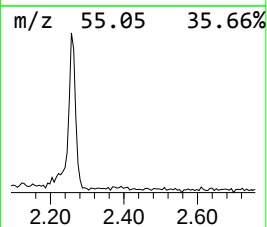
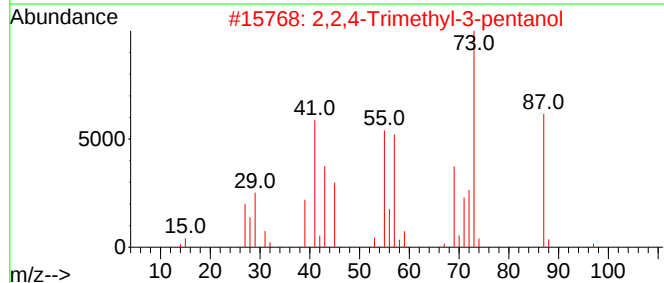
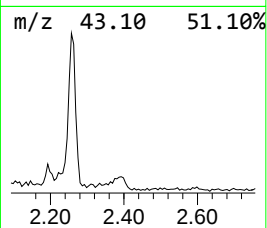
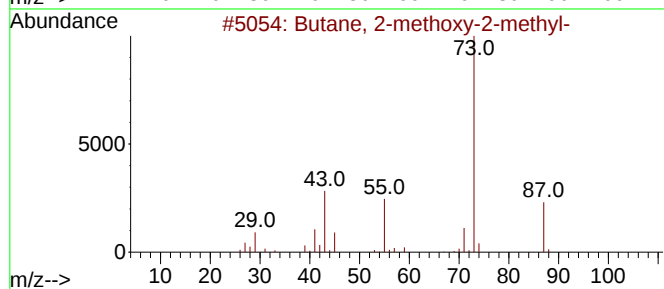
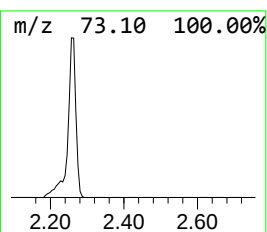
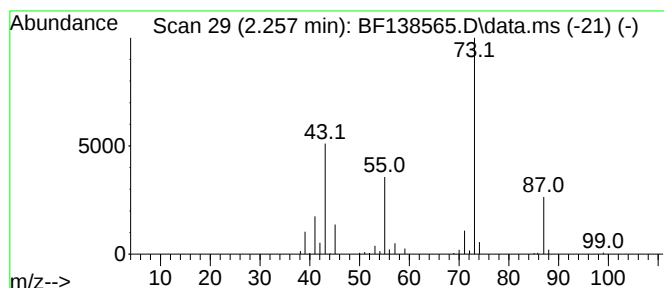
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	3.06 ng	150611	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25



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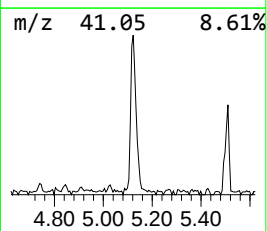
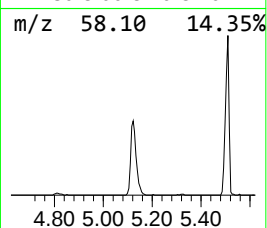
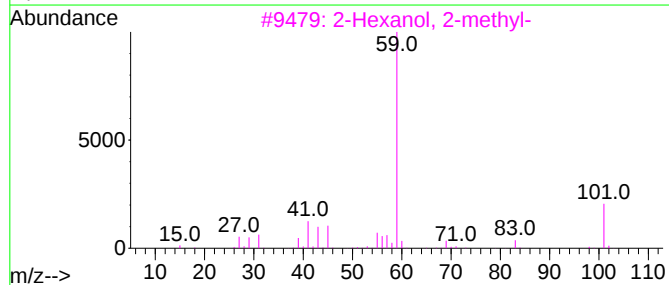
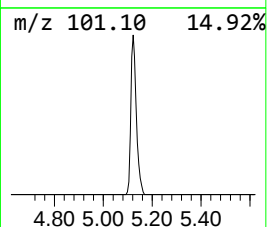
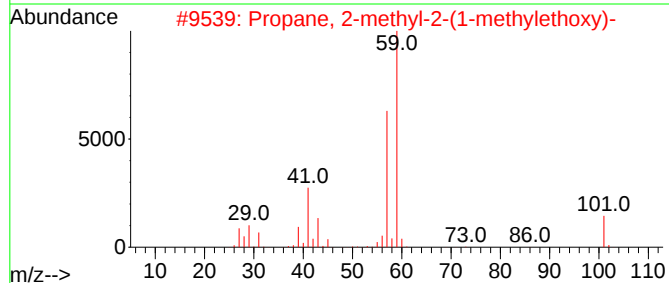
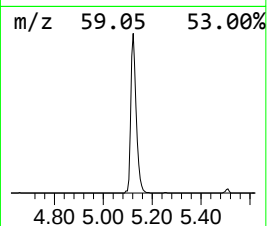
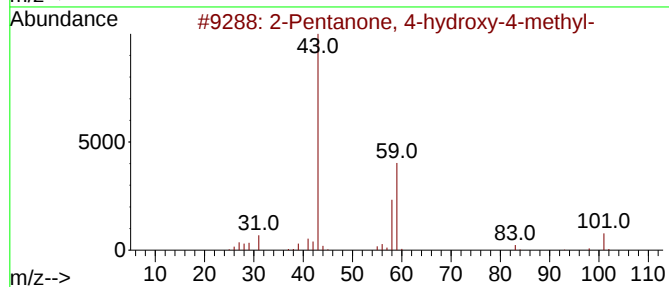
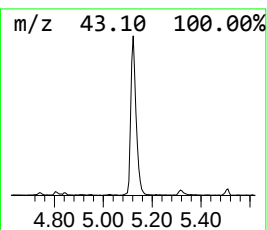
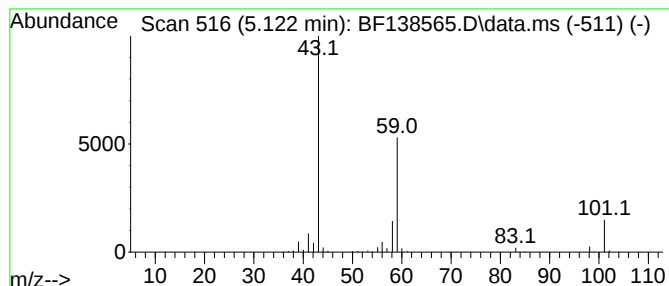
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	8.04 ng	395930	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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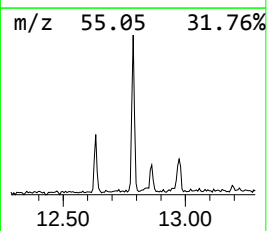
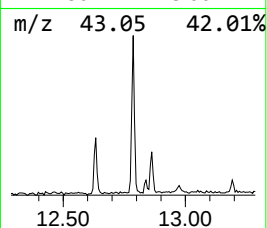
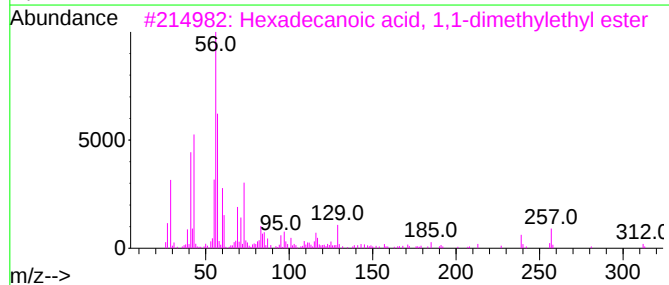
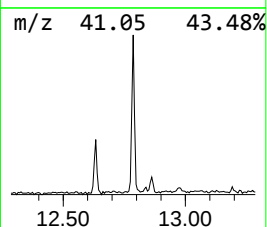
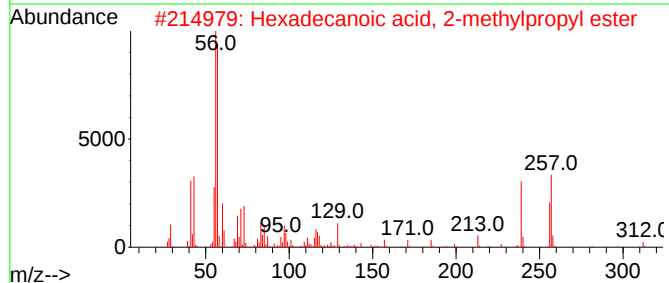
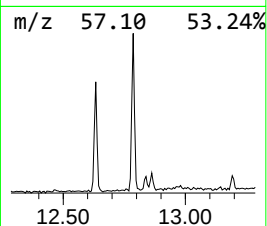
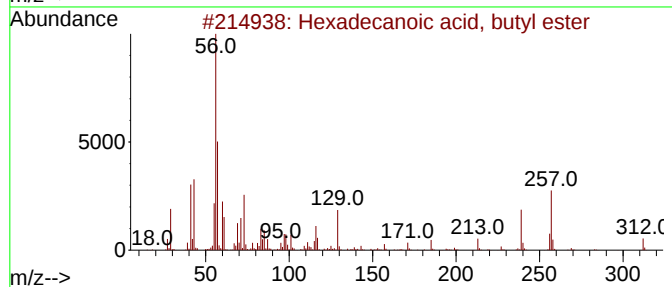
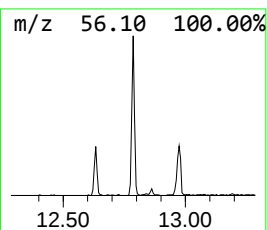
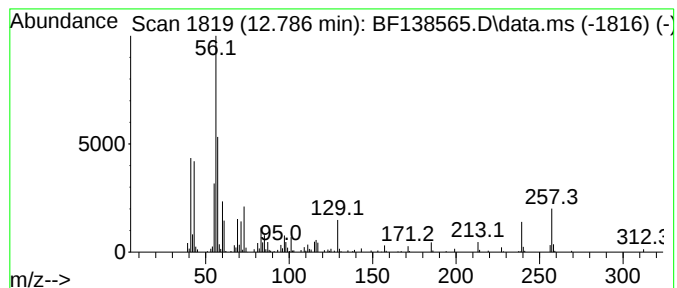
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	3.98 ng	208136	Chrysene-d12	14.021

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	70
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	55
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38



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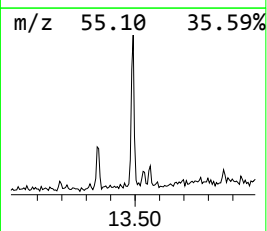
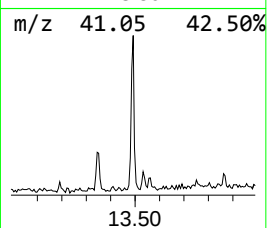
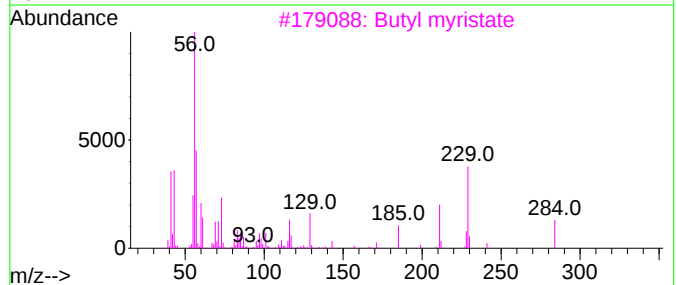
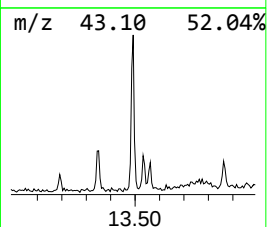
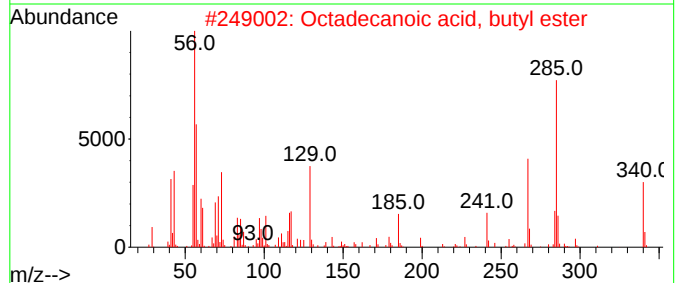
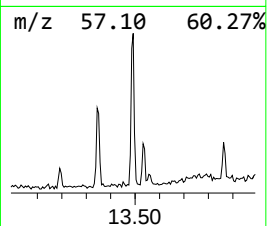
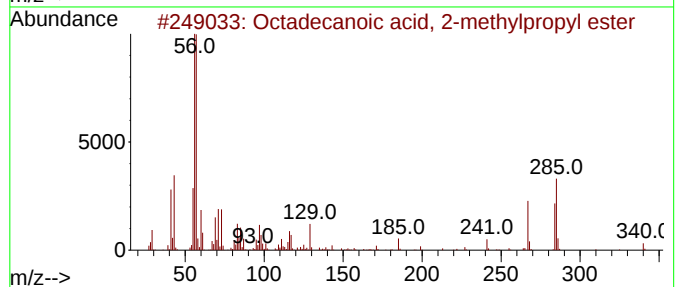
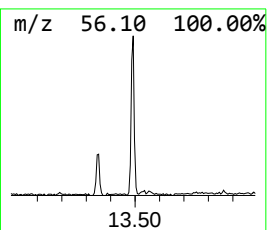
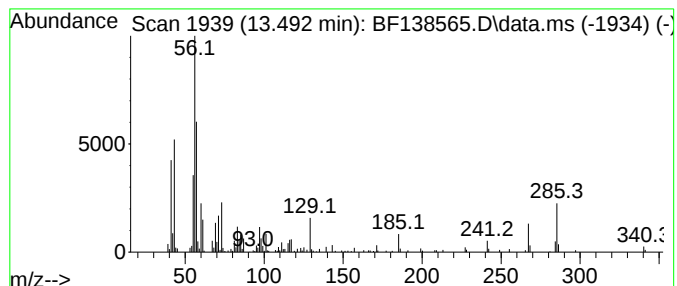
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Peak Number 4 Octadecanoic acid, 2-methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	3.00 ng	156793	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	89
2			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	83
3			Butyl myristate	284	C18H36O2	000110-36-1	59
4			Octadecanoic acid	284	C18H36O2	000057-11-4	38
5			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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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	3.1	ng	150611	1	6.869	984819	20.0
2-Pentanone, 4-...	5.122	8.0	ng	395930	1	6.869	984819	20.0
Hexadecanoic ac...	12.786	4.0	ng	208136	5	14.021	1046810	20.0
Octadecanoic ac...	13.492	3.0	ng	156793	5	14.021	1046810	20.0