

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
 Data File : BF138543.D
 Acq On : 12 Jul 2024 13:23
 Operator : CG\JU
 Sample : PB161988BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB161988BL

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: BF138543.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.281	26	33	38	rVB	90396	120341	2.43%	0.390%
2	5.122	512	516	528	rVB	209331	319645	6.45%	1.036%
3	5.510	576	582	585	rBV	3872680	3971477	80.19%	12.866%
4	6.504	745	751	754	rBV	3442941	4118282	83.15%	13.342%
5	6.863	808	812	816	rBV	1045030	839023	16.94%	2.718%
6	7.434	902	909	911	rBV	2190252	2771062	55.95%	8.977%
7	8.145	1025	1030	1033	rBV	1245578	1138090	22.98%	3.687%
8	9.222	1206	1213	1216	rBV	4519442	4859290	98.11%	15.742%
9	9.898	1322	1328	1332	rBV	1551637	1336931	26.99%	4.331%
10	10.692	1456	1463	1466	rBV	3001078	3024204	61.06%	9.797%
11	11.386	1577	1581	1584	rBV	1727390	1397472	28.22%	4.527%
12	12.633	1789	1793	1796	rVB	84478	67537	1.36%	0.219%
13	12.786	1815	1819	1822	rBV	254414	194026	3.92%	0.629%
14	12.975	1845	1851	1854	rBV	4798728	4952855	100.00%	16.045%
15	13.492	1933	1939	1942	rBV	150770	136877	2.76%	0.443%
16	14.021	2025	2029	2032	rBV	1068002	909580	18.36%	2.947%
17	15.486	2273	2278	2292	rVB	538641	710898	14.35%	2.303%

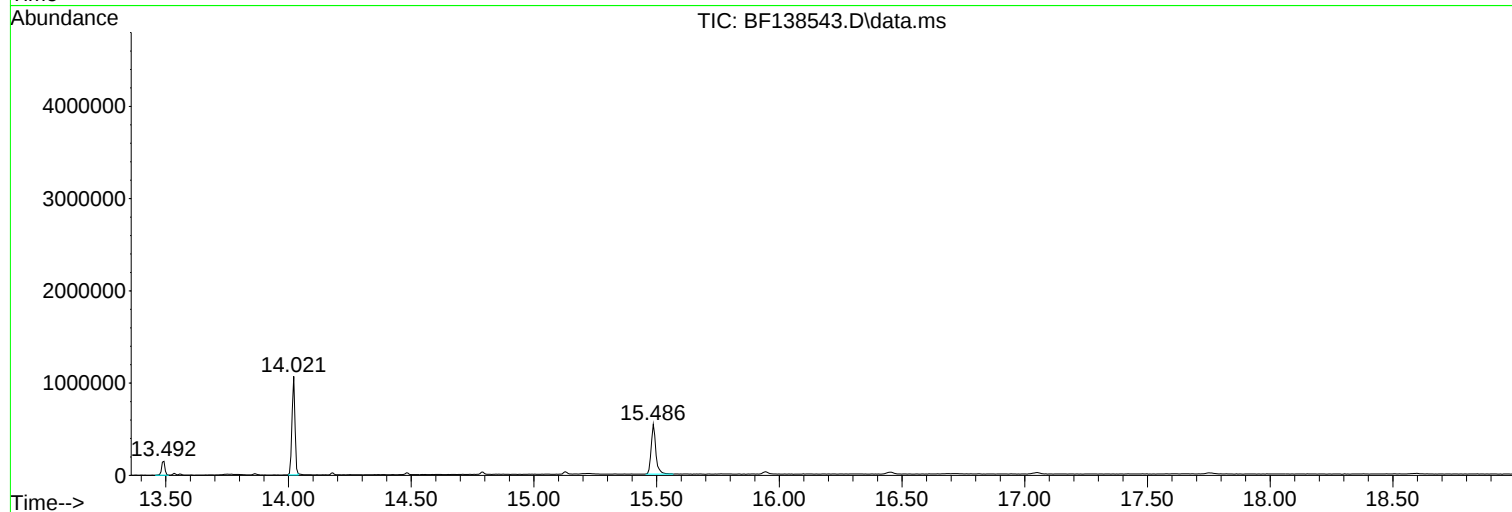
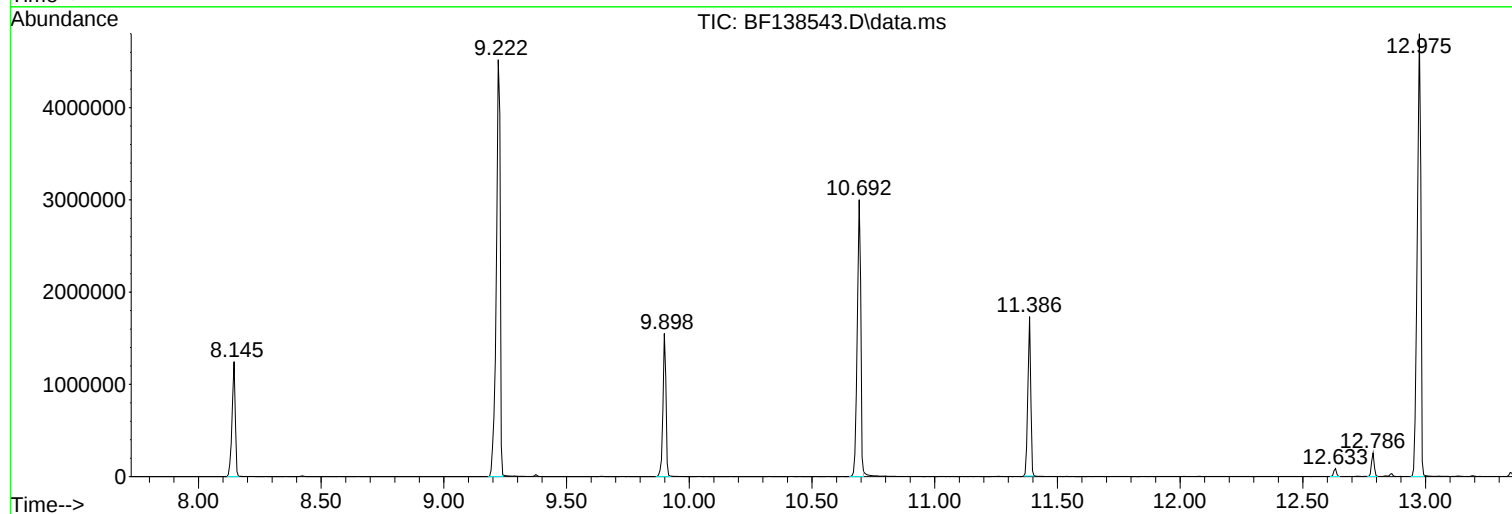
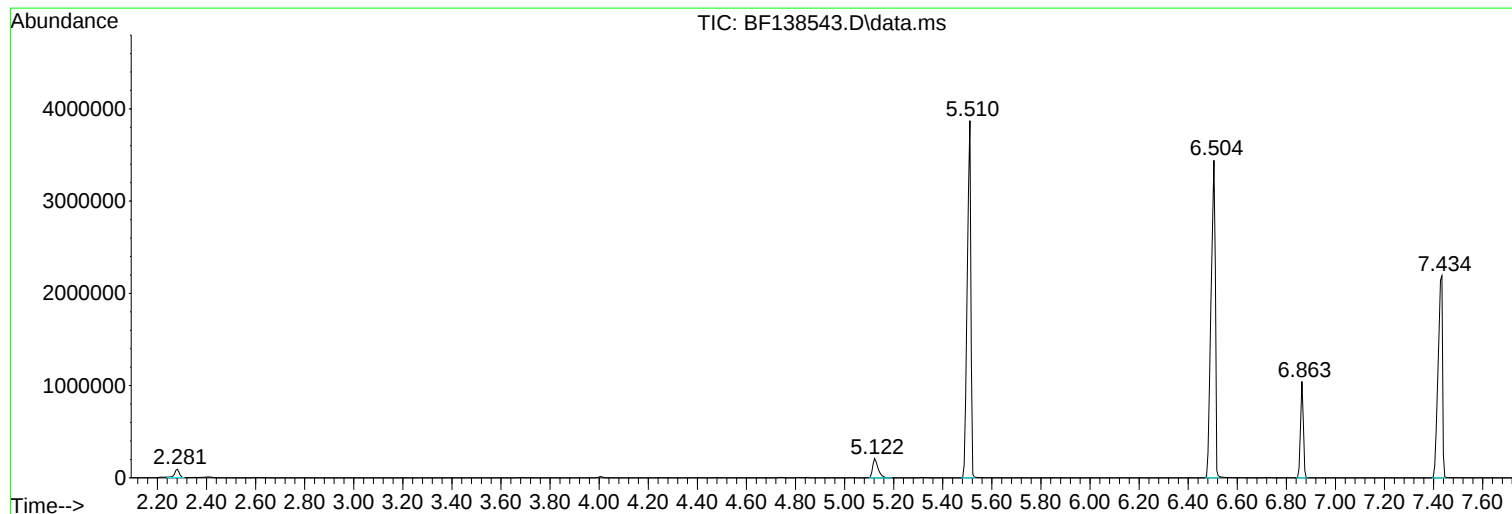
Sum of corrected areas: 30867590

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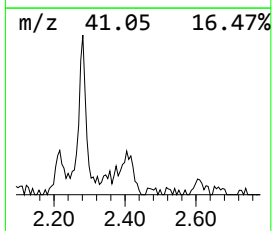
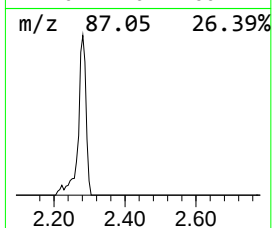
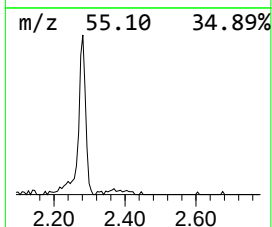
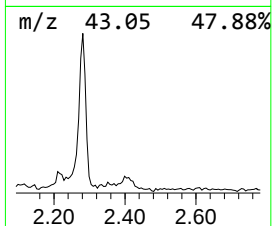
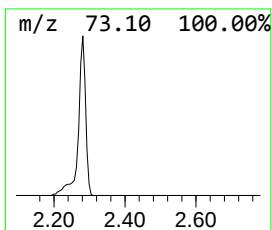
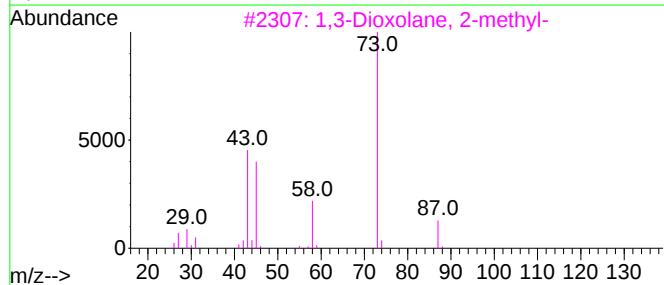
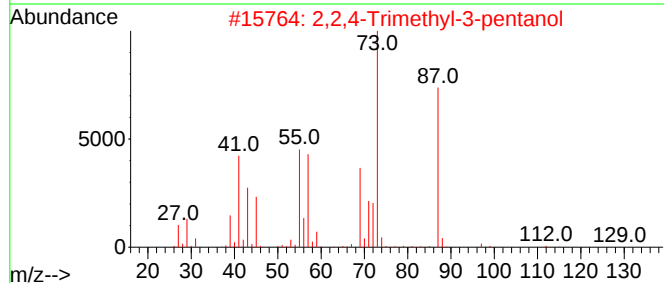
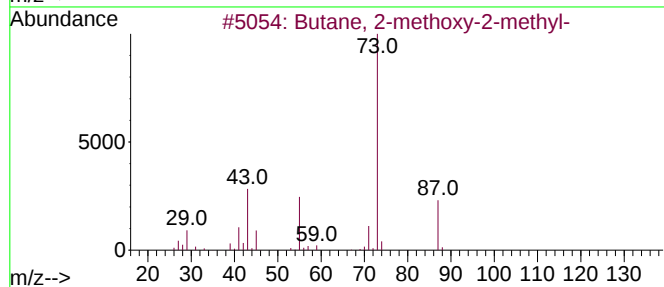
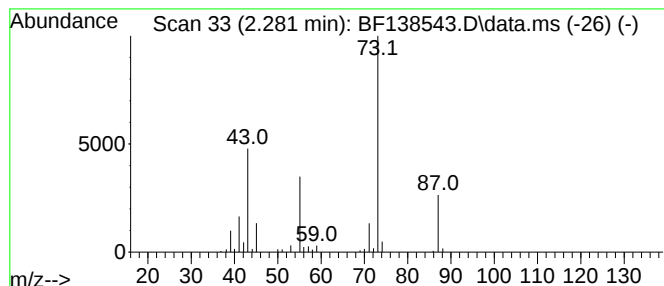
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	2.87 ng	120341	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			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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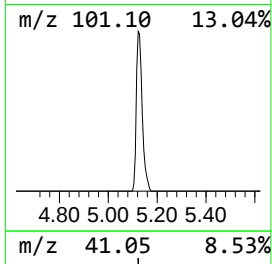
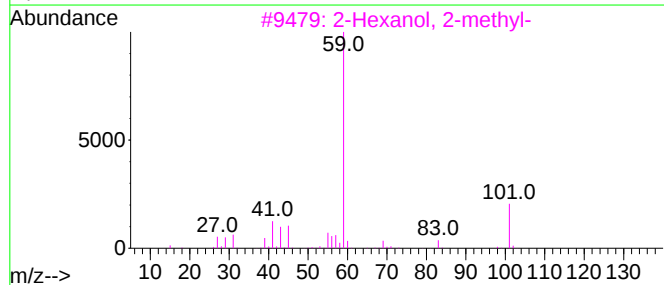
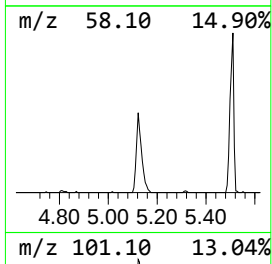
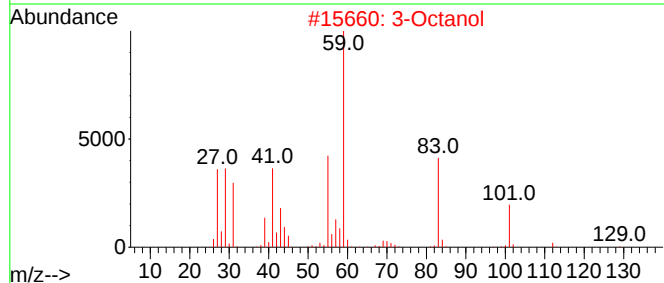
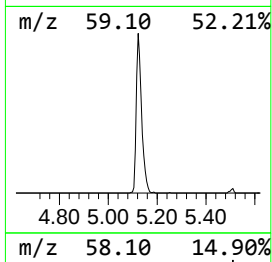
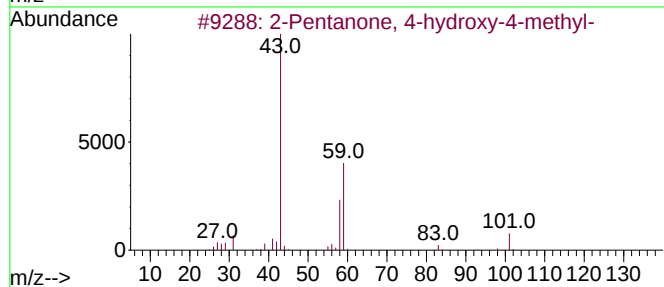
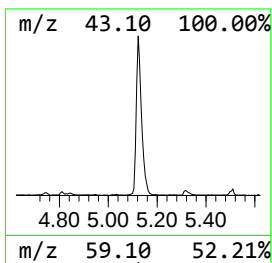
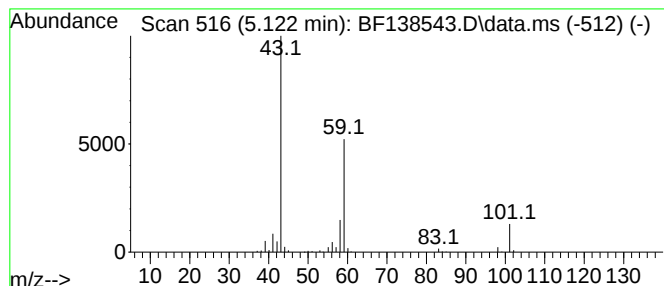
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.122	7.62 ng	319645	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	64
2	3-Octanol		130	C8H18O	000589-98-0	33
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	12



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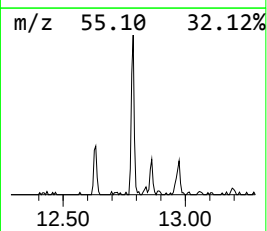
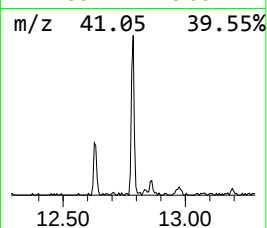
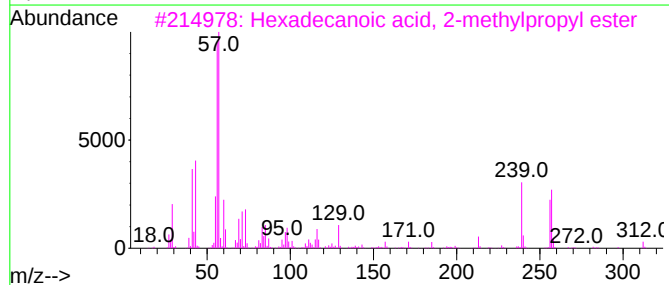
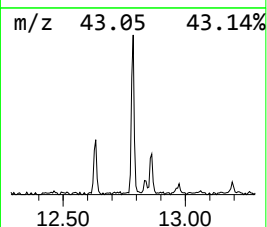
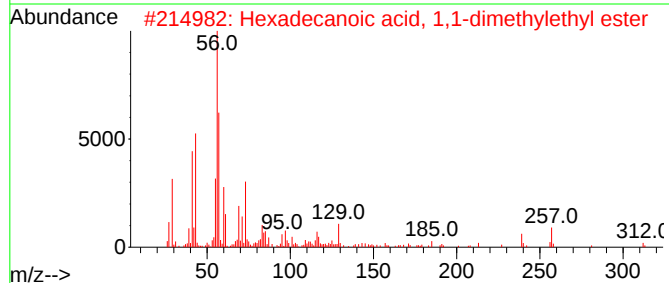
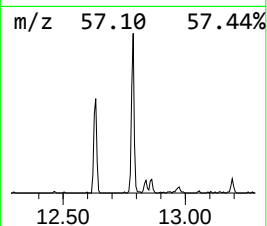
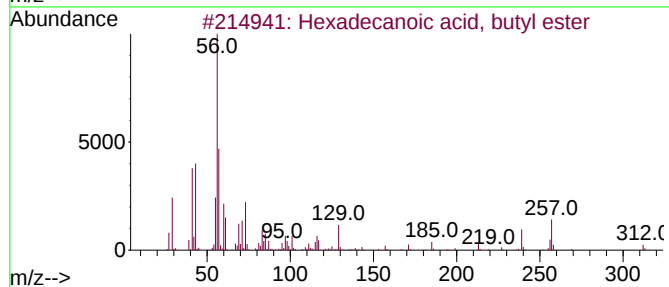
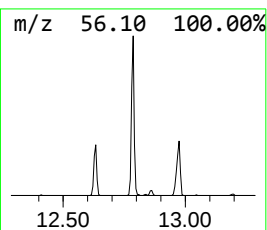
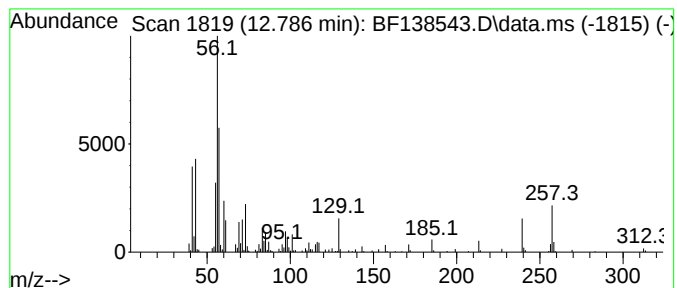
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Peak Number 3 Hexadecanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	4.27 ng	194026	Chrysene-d12	14.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	96
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
4			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5			Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27



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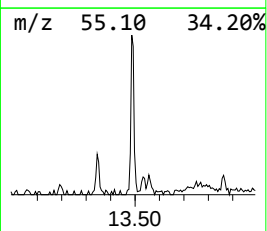
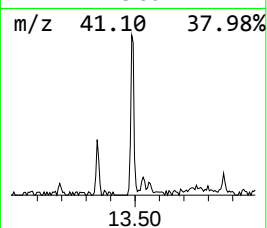
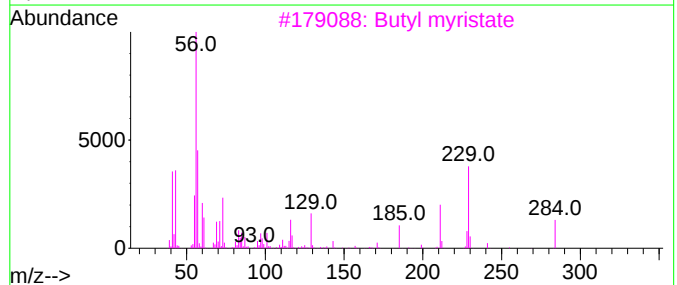
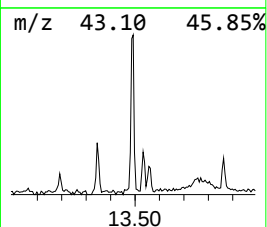
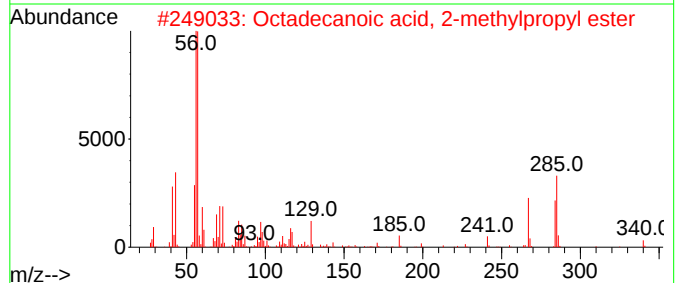
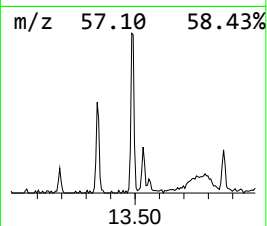
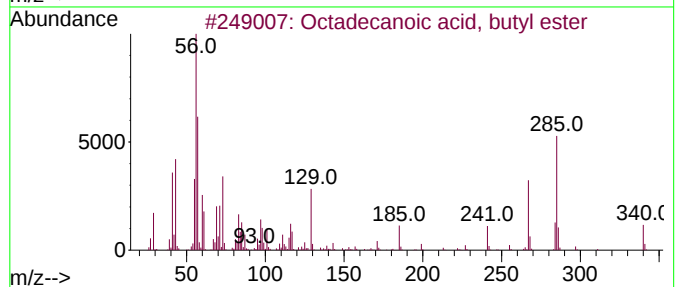
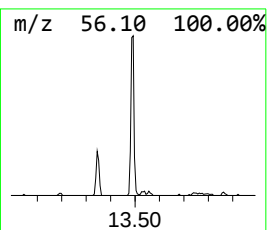
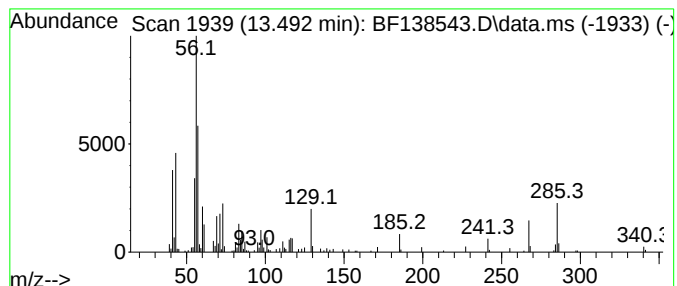
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Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	3.01 ng	136877	Chrysene-d12	14.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2			Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	90
3			Butyl myristate	284	C18H36O2	000110-36-1	64
4			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5			2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.281	2.9	ng	120341	1	6.863	839023	20.0
2-Pentanone, 4-...	5.122	7.6	ng	319645	1	6.863	839023	20.0
Hexadecanoic ac...	12.786	4.3	ng	194026	5	14.022	909580	20.0
Octadecanoic ac...	13.492	3.0	ng	136877	5	14.022	909580	20.0