

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070224\
 Data File : BF138422.D
 Acq On : 02 Jul 2024 11:40
 Operator : CG\JU
 Sample : PB161833BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB161833BL

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-BF062824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138422.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	14	29	35	rVB	123075	197614	3.14%	0.500%
2	2.363	41	47	56	rVB	66511	88160	1.40%	0.223%
3	5.116	511	515	527	rVB	395165	599905	9.53%	1.516%
4	5.516	577	583	586	rBV	5439877	5542608	88.08%	14.010%
5	6.510	747	752	755	rBV	4825291	5777364	91.81%	14.603%
6	6.875	810	814	817	rBV	1429919	1270449	20.19%	3.211%
7	7.433	903	909	913	rBV	3170186	3889020	61.80%	9.830%
8	8.151	1026	1031	1035	rBV	1846495	1762204	28.00%	4.454%
9	9.227	1208	1214	1217	rBV	5588730	6292475	100.00%	15.906%
10	9.904	1323	1329	1333	rBV	2073262	2018758	32.08%	5.103%
11	10.698	1457	1464	1467	rBV	3643844	3446639	54.77%	8.712%
12	11.392	1578	1582	1585	rBV	2357587	1901676	30.22%	4.807%
13	12.639	1791	1794	1798	rVB	84036	64372	1.02%	0.163%
14	12.792	1817	1820	1824	rBV	393730	295671	4.70%	0.747%
15	12.980	1847	1852	1855	rBV	4464649	4366439	69.39%	11.037%
16	13.498	1937	1940	1944	rBV	212545	164321	2.61%	0.415%
17	14.027	2026	2030	2039	rBV	1074997	963260	15.31%	2.435%
18	15.492	2274	2279	2292	rBV	705521	920589	14.63%	2.327%

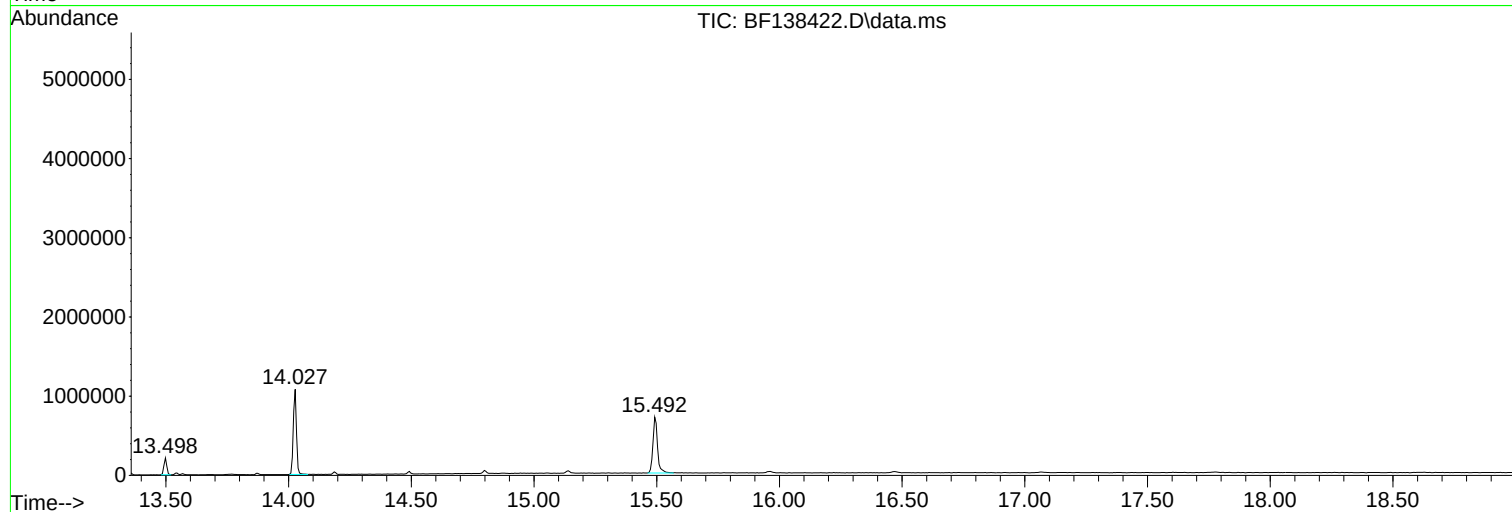
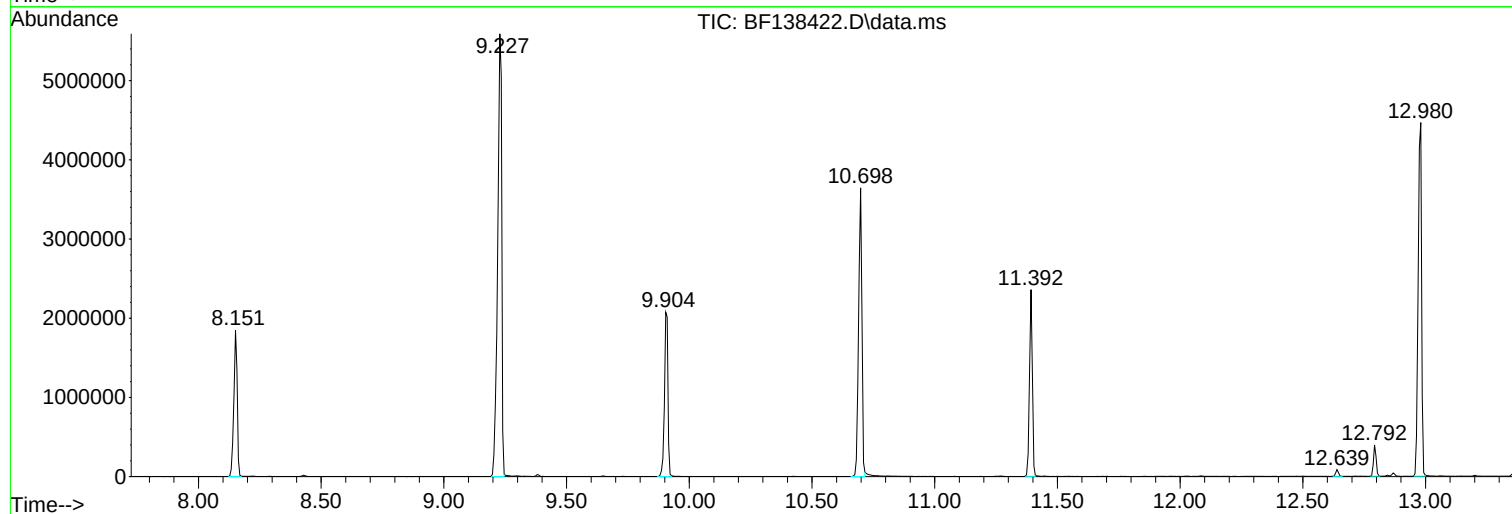
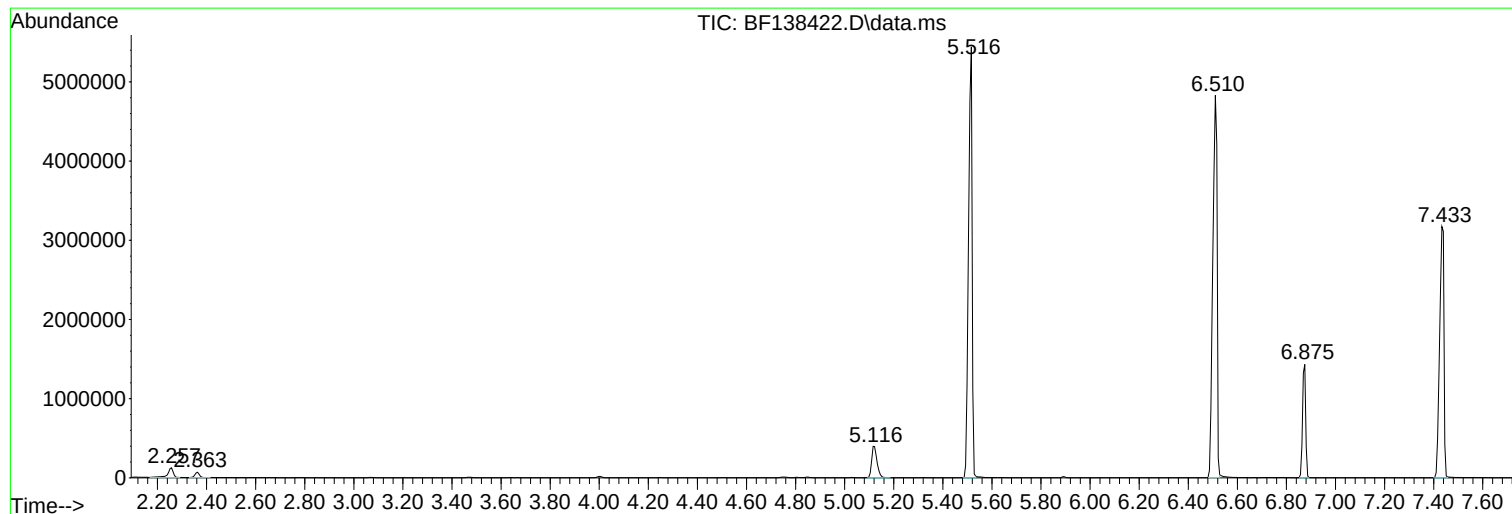
Sum of corrected areas: 39561524

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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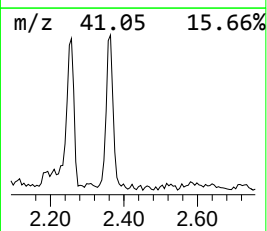
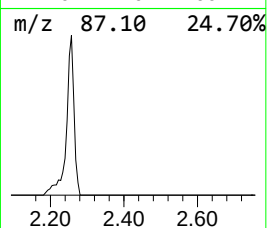
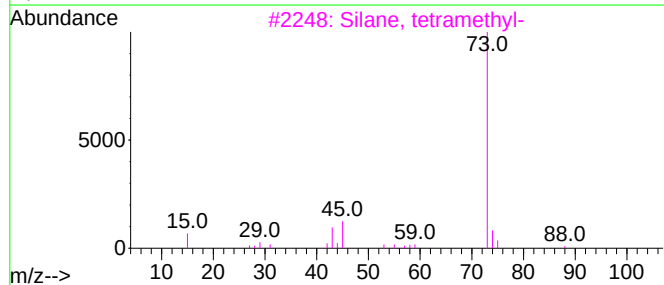
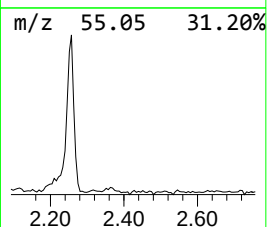
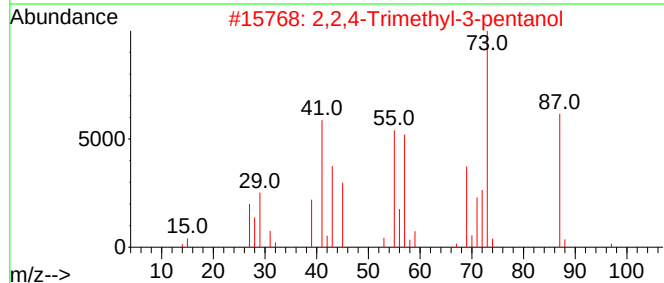
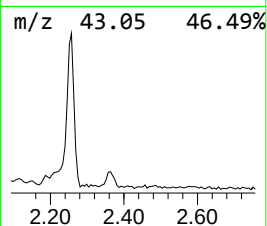
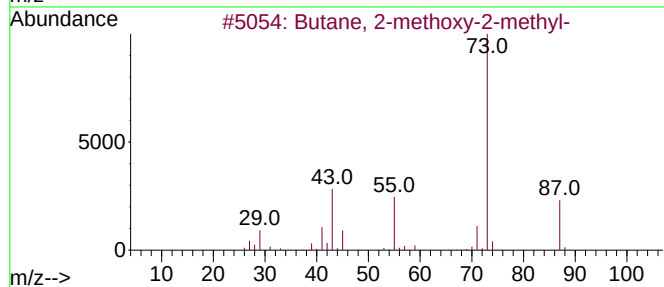
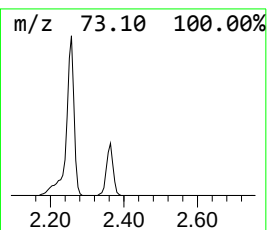
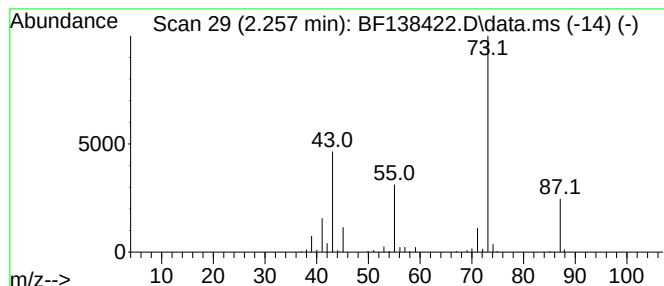
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.257	3.11 ng	197614	1,4-Dichlorobenzene-d4	6.875

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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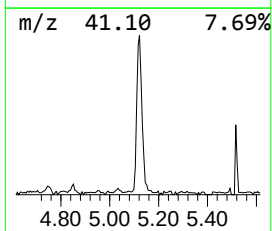
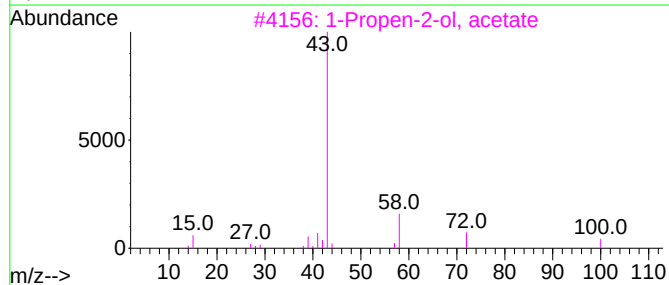
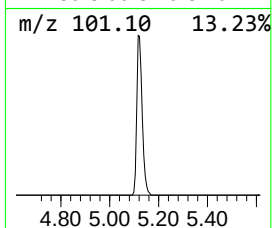
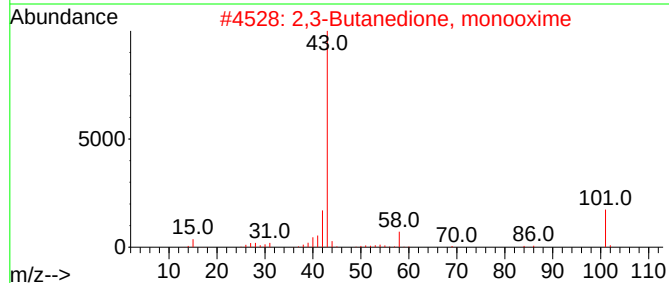
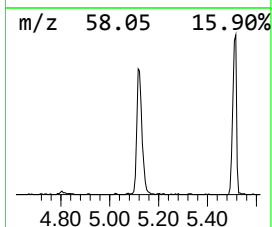
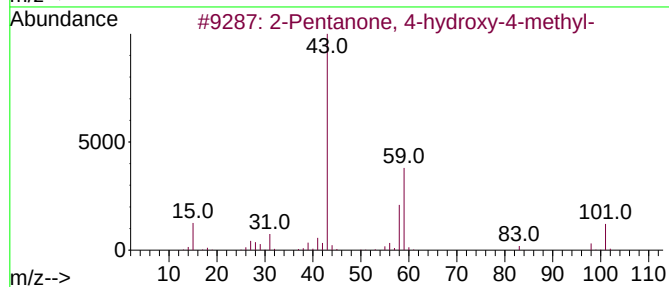
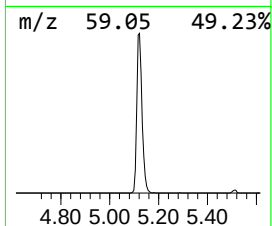
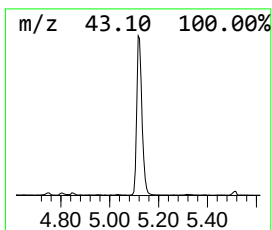
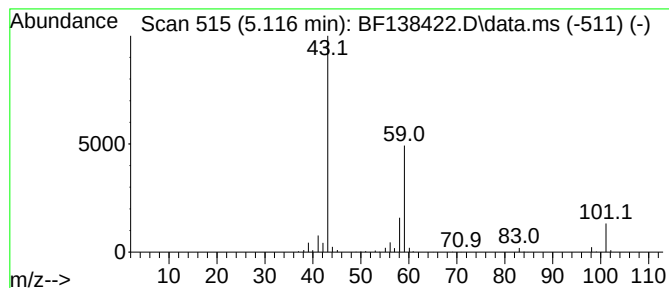
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.116	9.44 ng	599905	1,4-Dichlorobenzene-d4			6.875
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
4	Allyl acetate		100	C5H8O2	000591-87-7	9
5	5-Oxohexanenitrile		111	C6H9NO	010412-98-3	9



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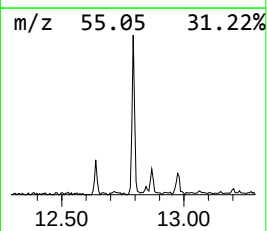
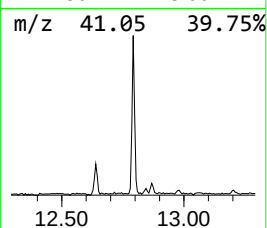
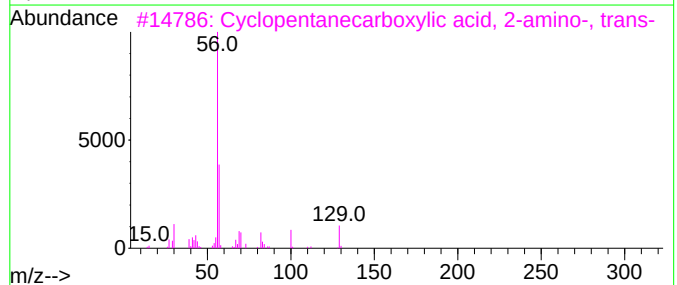
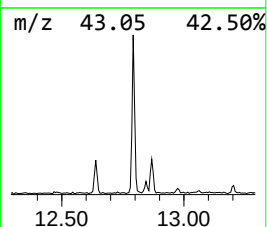
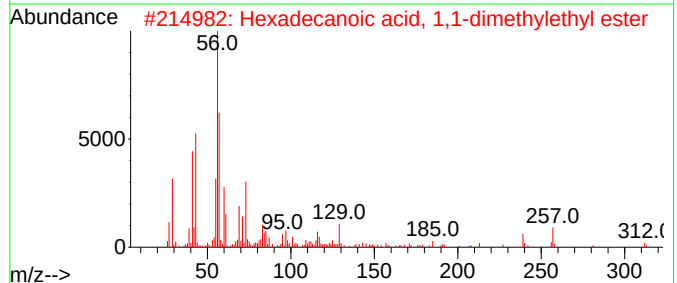
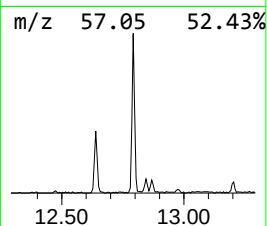
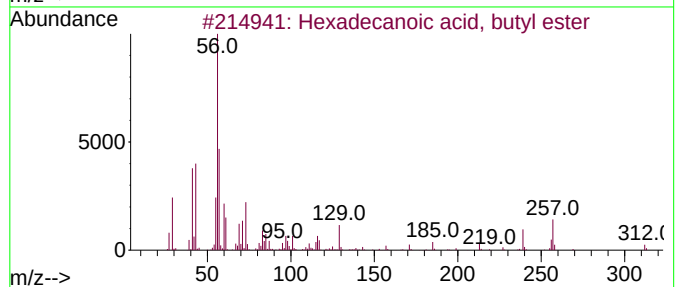
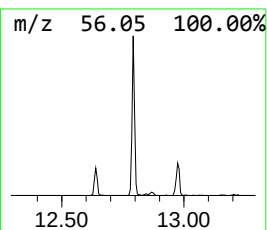
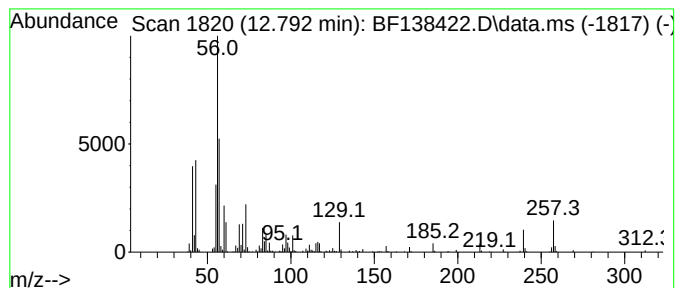
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Peak Number 3 Hexadecanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.792	6.14 ng	295671	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5			Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35



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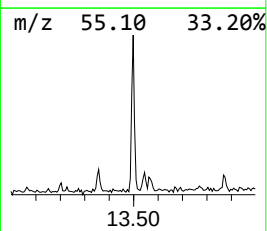
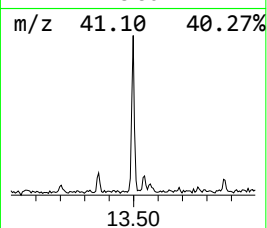
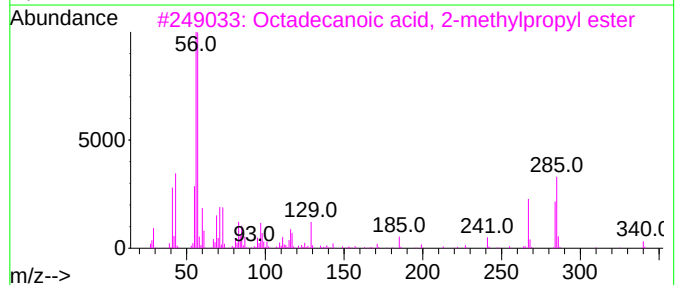
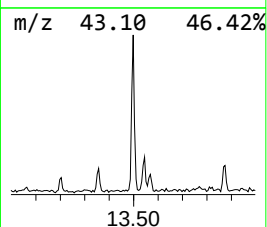
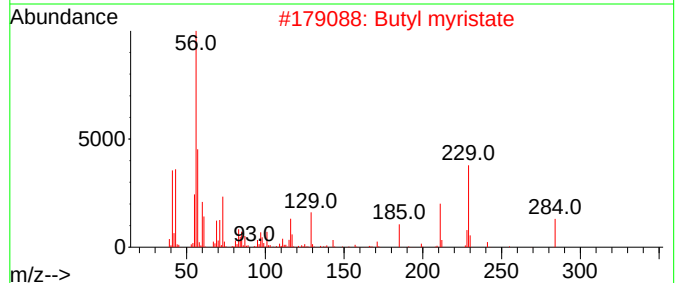
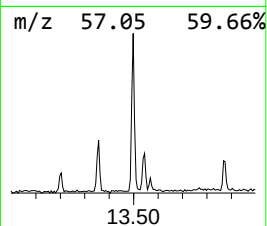
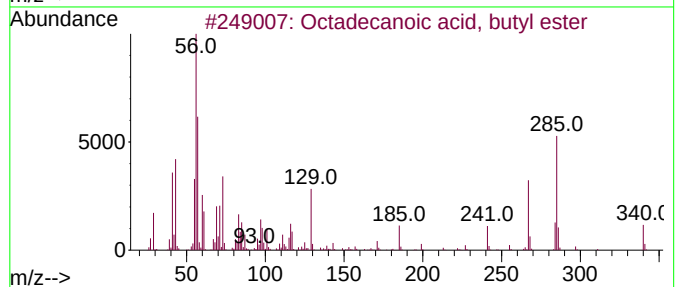
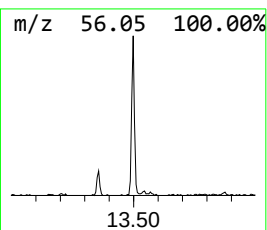
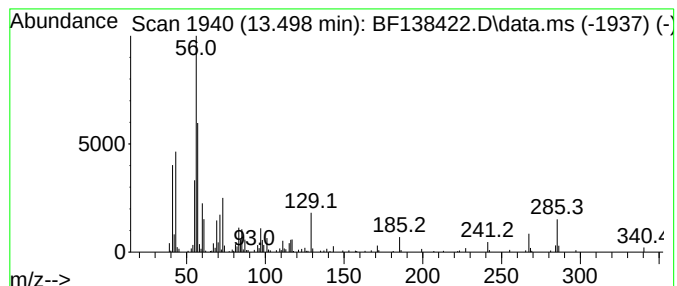
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Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	3.41 ng	164321	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	97
2			Butyl myristate	284	C18H36O2	000110-36-1	78
3			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	45
4			5-Methyl-2-hexanol, chlorodifluo...	228	C9H15ClF2O2	1010376-27-1	38
5			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.257	3.1	ng	197614	1	6.875	1270450	20.0
2-Pentanone, 4-...	5.116	9.4	ng	599905	1	6.875	1270450	20.0
Hexadecanoic ac...	12.792	6.1	ng	295671	5	14.027	963260	20.0
Octadecanoic ac...	13.498	3.4	ng	164321	5	14.027	963260	20.0