

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070524\
 Data File : BF138463.D
 Acq On : 05 Jul 2024 12:22
 Operator : CG\JU
 Sample : PB161894BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB161894BL

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: BF138463.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	18	26	36	rVB	63877	93950	2.12%	0.340%
2	5.116	506	515	524	rBV	221695	312762	7.06%	1.133%
3	5.510	577	582	585	rBV	3841123	3820884	86.24%	13.845%
4	6.510	747	752	755	rBV	3497609	4044721	91.29%	14.656%
5	6.869	810	813	817	rBV	921823	815662	18.41%	2.955%
6	7.275	878	882	888	rBV2	42362	45936	1.04%	0.166%
7	7.434	903	909	912	rBV	2251016	2652802	59.88%	9.612%
8	8.151	1026	1031	1034	rBV	1186531	1110799	25.07%	4.025%
9	9.234	1209	1215	1218	rVB	4111450	4430503	100.00%	16.053%
10	9.910	1324	1330	1333	rBV	1479291	1282350	28.94%	4.646%
11	10.451	1419	1422	1428	rVB3	37496	45495	1.03%	0.165%
12	10.698	1458	1464	1468	rBV	2662419	2570661	58.02%	9.315%
13	11.392	1578	1582	1585	rBV	1341685	1248152	28.17%	4.523%
14	12.798	1817	1821	1824	rBV	139782	113077	2.55%	0.410%
15	12.981	1847	1852	1856	rBV	3600228	3698993	83.49%	13.403%
16	13.504	1937	1941	1945	rBV	78382	78567	1.77%	0.285%
17	14.033	2027	2031	2034	rBV	740399	651265	14.70%	2.360%
18	15.504	2276	2281	2289	rBV	474544	581823	13.13%	2.108%

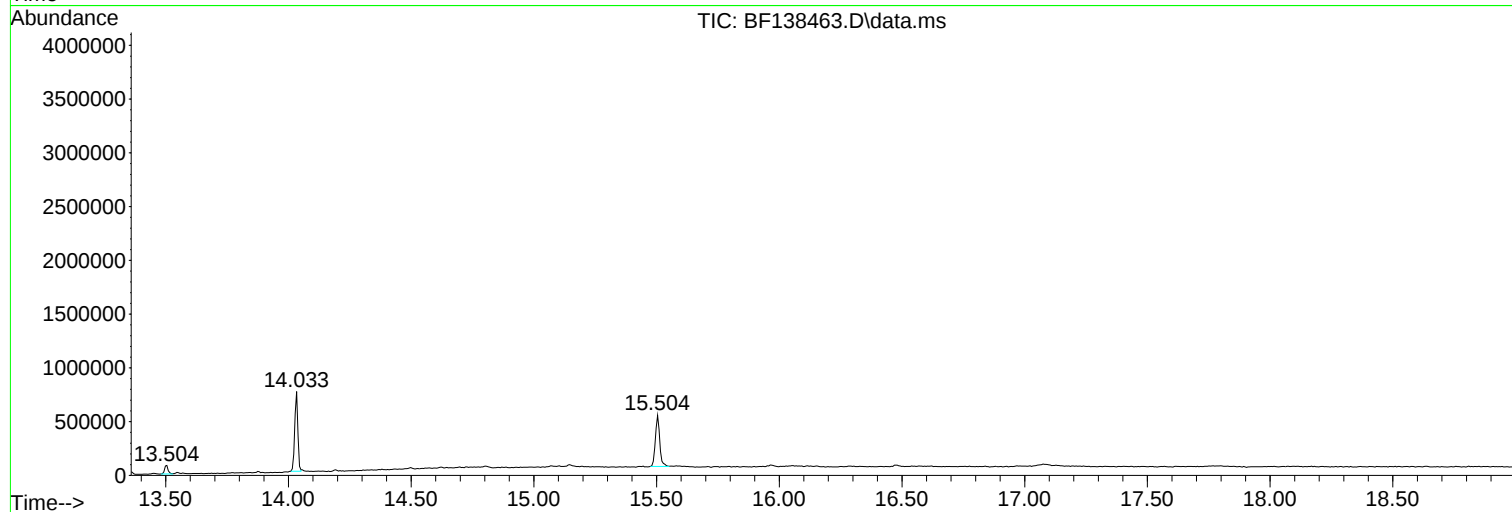
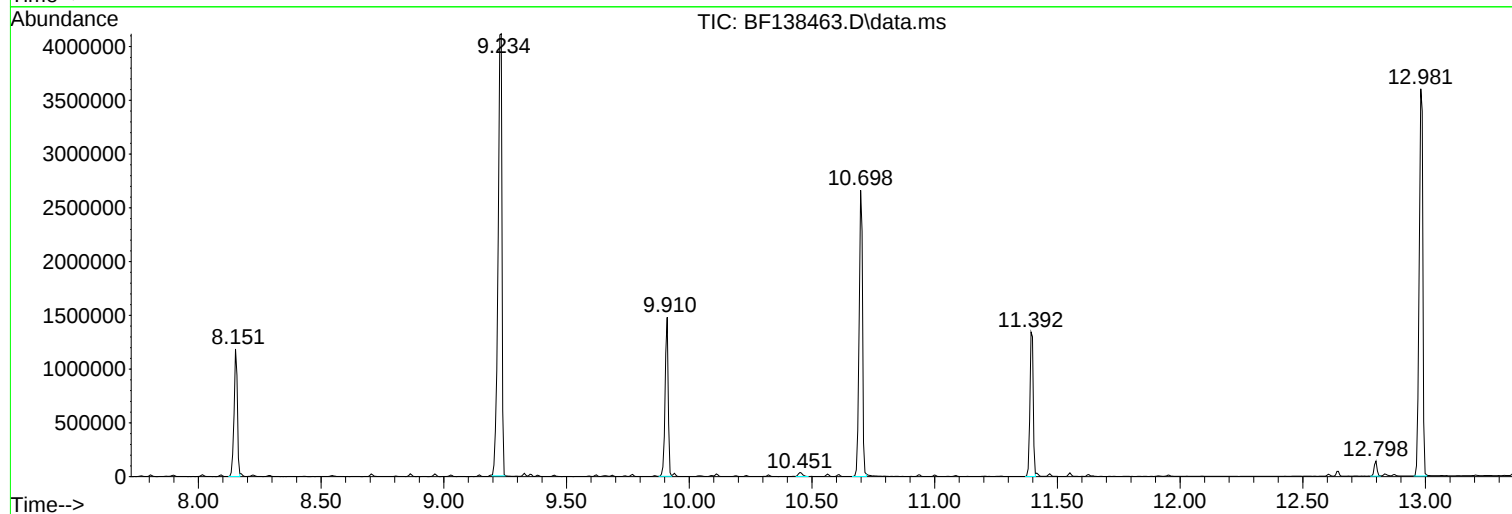
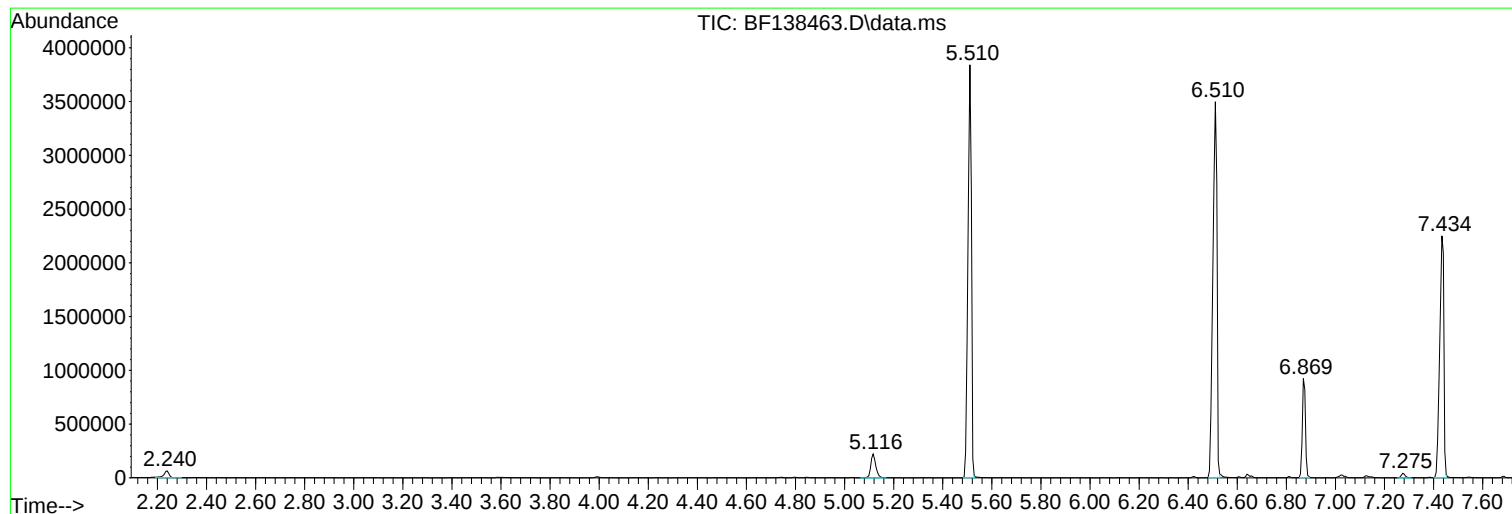
Sum of corrected areas: 27598402

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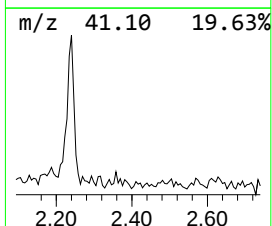
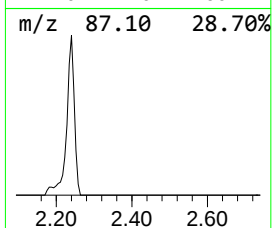
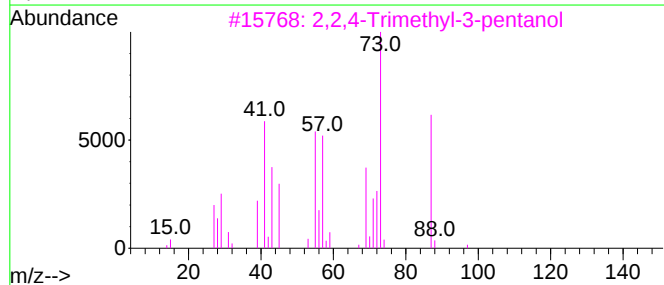
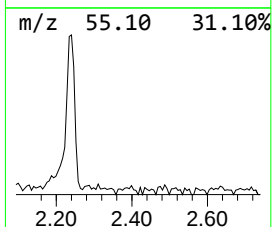
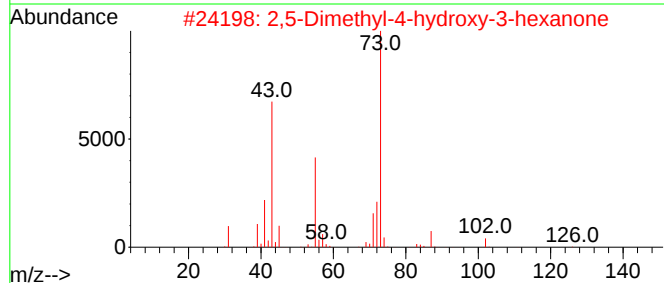
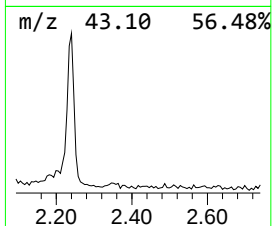
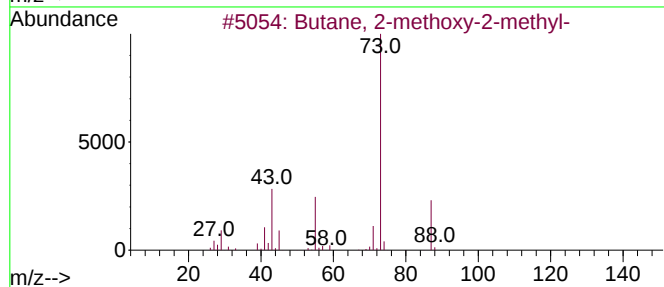
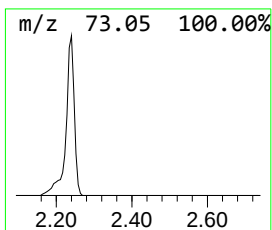
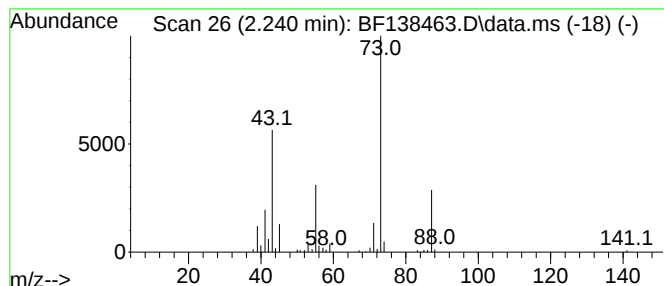
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.240	2.30 ng	93950	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	90
2		2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	53
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28



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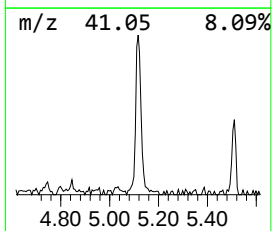
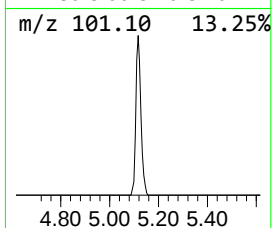
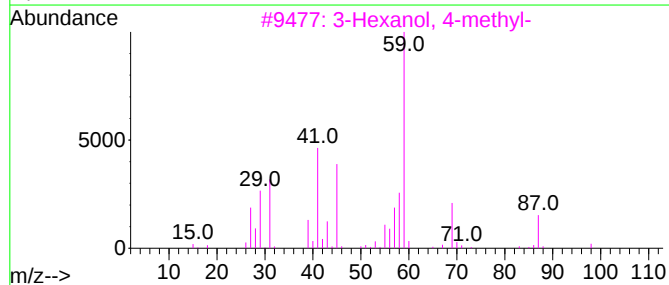
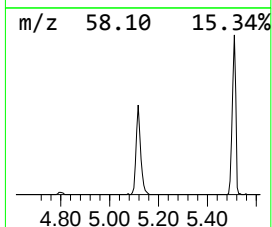
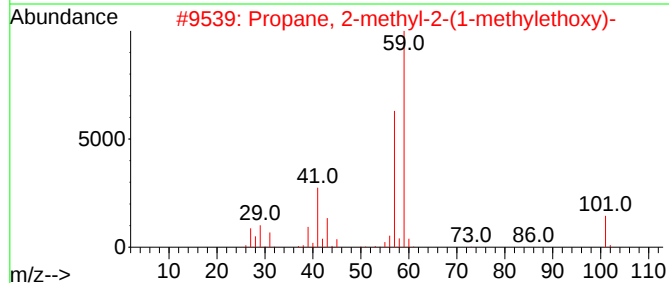
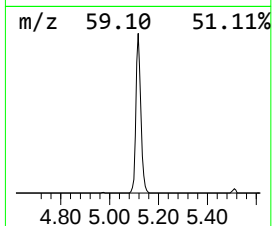
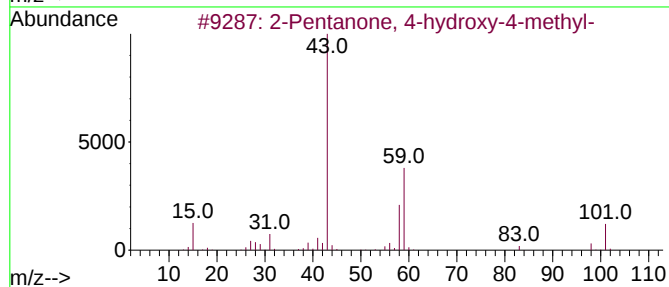
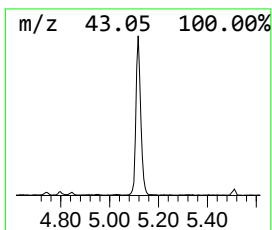
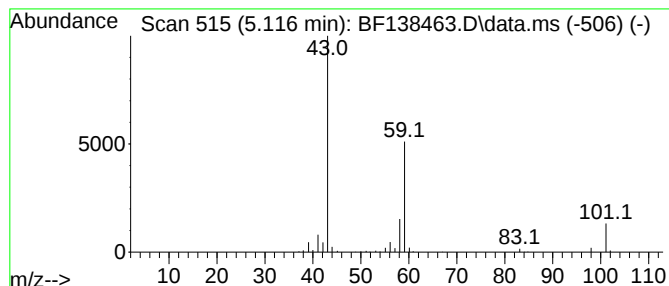
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	7.67 ng	312762	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	42		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
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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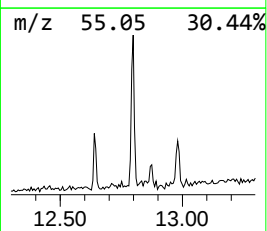
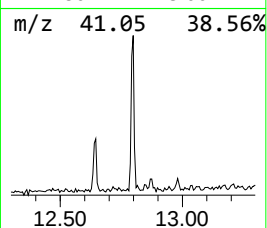
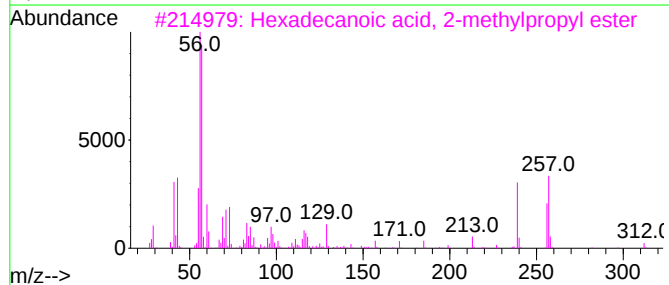
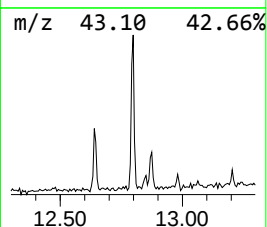
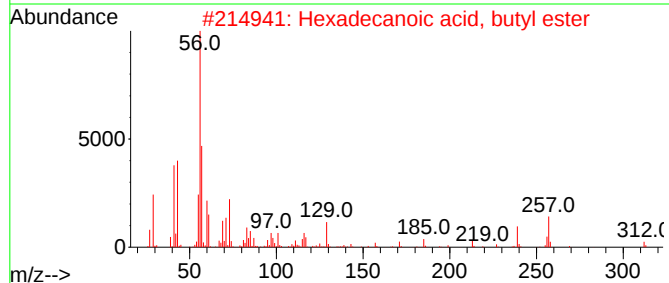
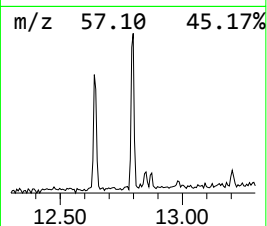
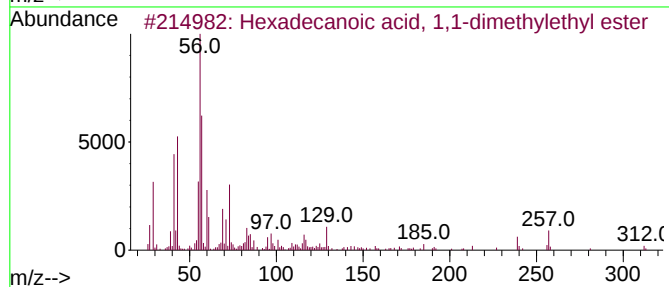
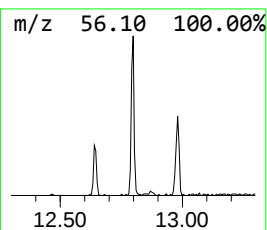
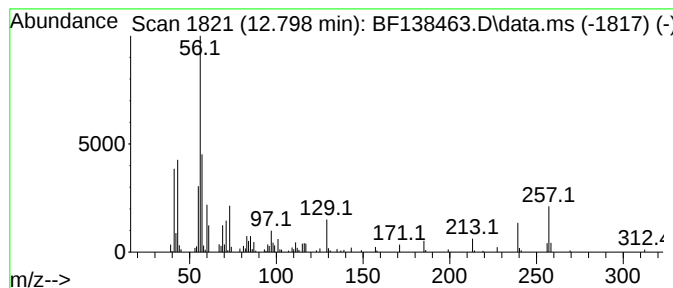
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Peak Number 3 Hexadecanoic acid, 1,1-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.798	3.47 ng	113077	Chrysene-d12	14.033

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	90
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	41
4			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37



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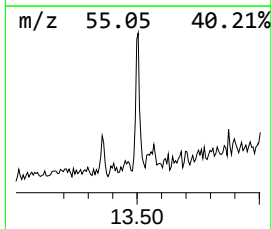
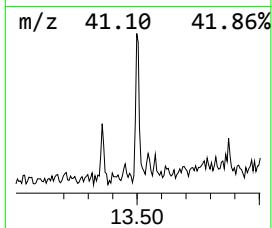
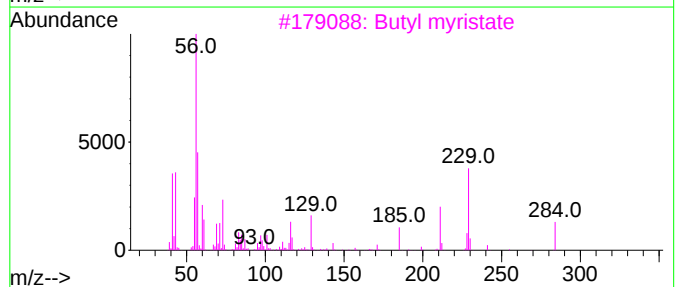
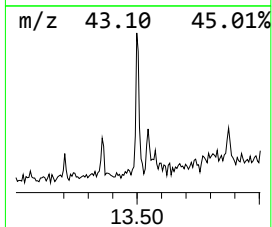
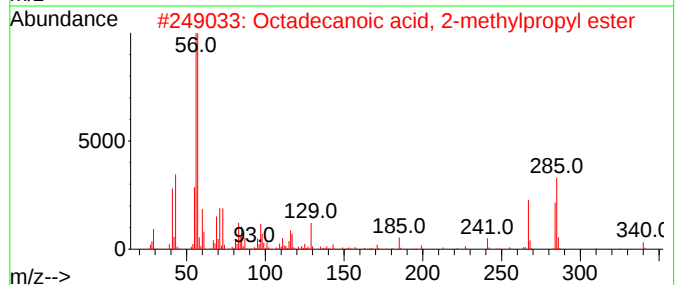
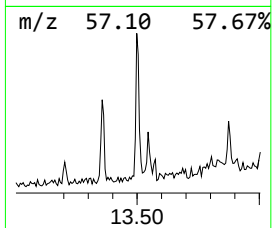
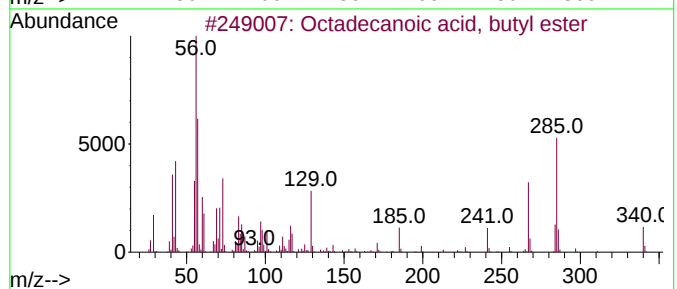
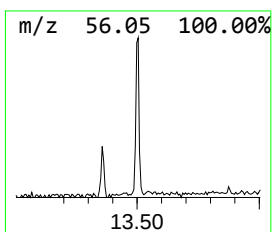
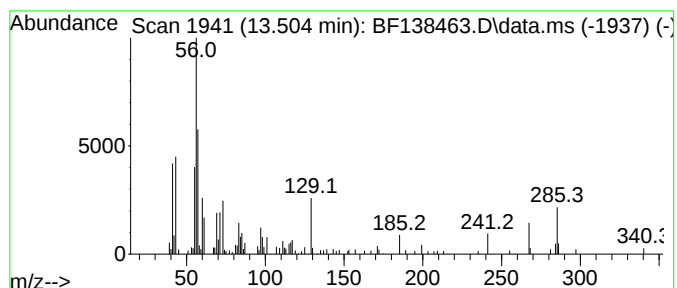
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Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	2.41 ng	78567	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	96
2			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	87
3			Butyl myristate	284	C18H36O2	000110-36-1	58
4			Nipecotic acid	129	C6H11NO2	000498-95-3	47
5			Piperidin-4-carboxylic acid	129	C6H11NO2	000498-94-2	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.240	2.3	ng	93950	1	6.869	815662	20.0
2-Pentanone, 4-...	5.116	7.7	ng	312762	1	6.869	815662	20.0
Hexadecanoic ac...	12.798	3.5	ng	113077	5	14.033	651265	20.0
Octadecanoic ac...	13.504	2.4	ng	78567	5	14.033	651265	20.0