

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070224\
 Data File : BF138419.D
 Acq On : 02 Jul 2024 10:12
 Operator : CG\JU
 Sample : PB161853BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB161853BL

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: BF138419.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	20	30	35	rVB	121596	187615	2.93%	0.466%
2	2.369	41	48	55	rVB	66877	86534	1.35%	0.215%
3	5.122	507	516	525	rBV	430514	615853	9.61%	1.531%
4	5.516	578	583	586	rBV	5683402	5582948	87.12%	13.879%
5	6.510	747	752	755	rBV	4870723	5822960	90.87%	14.475%
6	6.875	810	814	817	rBV	1469308	1279983	19.97%	3.182%
7	7.439	903	910	913	rBV	3329181	3955220	61.72%	9.832%
8	8.151	1026	1031	1035	rBV	1834008	1794874	28.01%	4.462%
9	9.233	1208	1215	1218	rBV	5685895	6408302	100.00%	15.930%
10	9.910	1324	1330	1333	rBV	2119855	2052661	32.03%	5.103%
11	10.698	1458	1464	1467	rBV	3611857	3579150	55.85%	8.897%
12	11.392	1578	1582	1585	rBV	2413022	1948258	30.40%	4.843%
13	12.639	1791	1794	1798	rBV	90564	69702	1.09%	0.173%
14	12.792	1817	1820	1824	rBV	403005	307757	4.80%	0.765%
15	12.980	1847	1852	1855	rBV	4413840	4454862	69.52%	11.074%
16	13.498	1937	1940	1944	rBV	217834	172009	2.68%	0.428%
17	14.027	2026	2030	2033	rBV	1111104	963864	15.04%	2.396%
18	15.492	2274	2279	2290	rBV	721786	944596	14.74%	2.348%

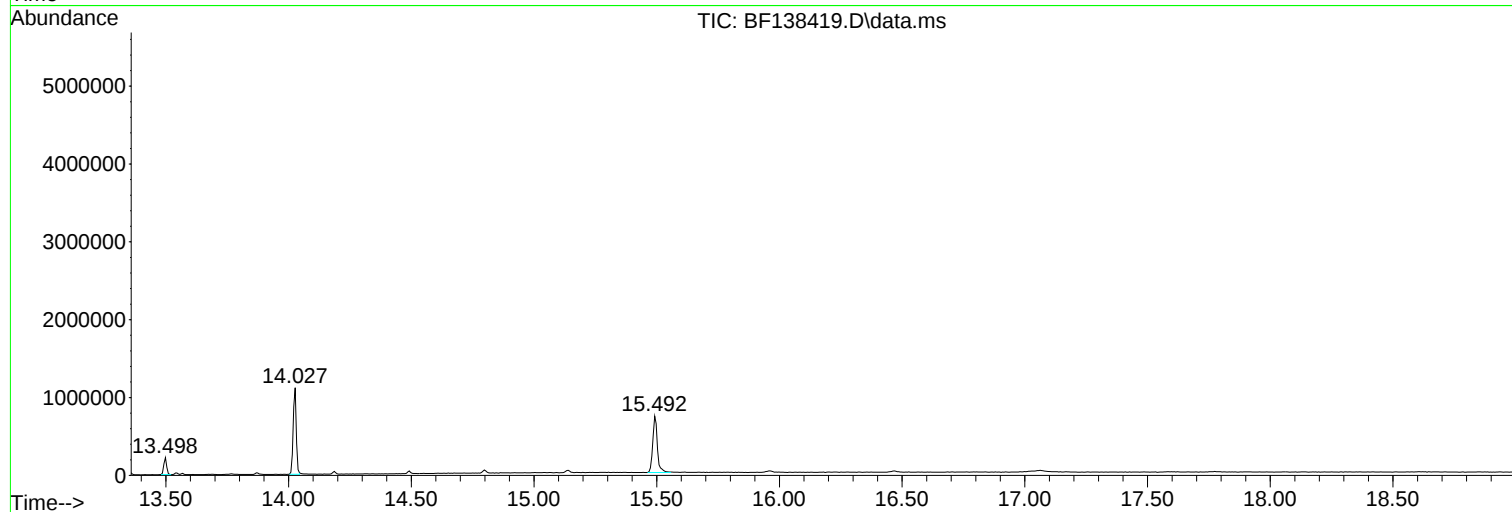
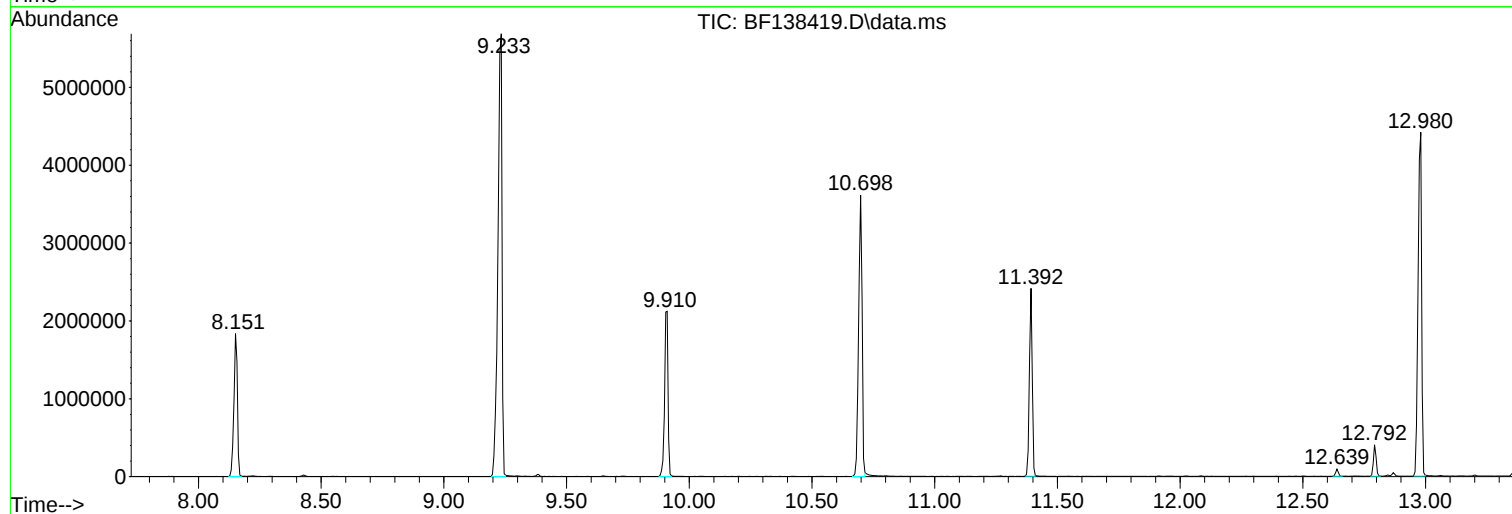
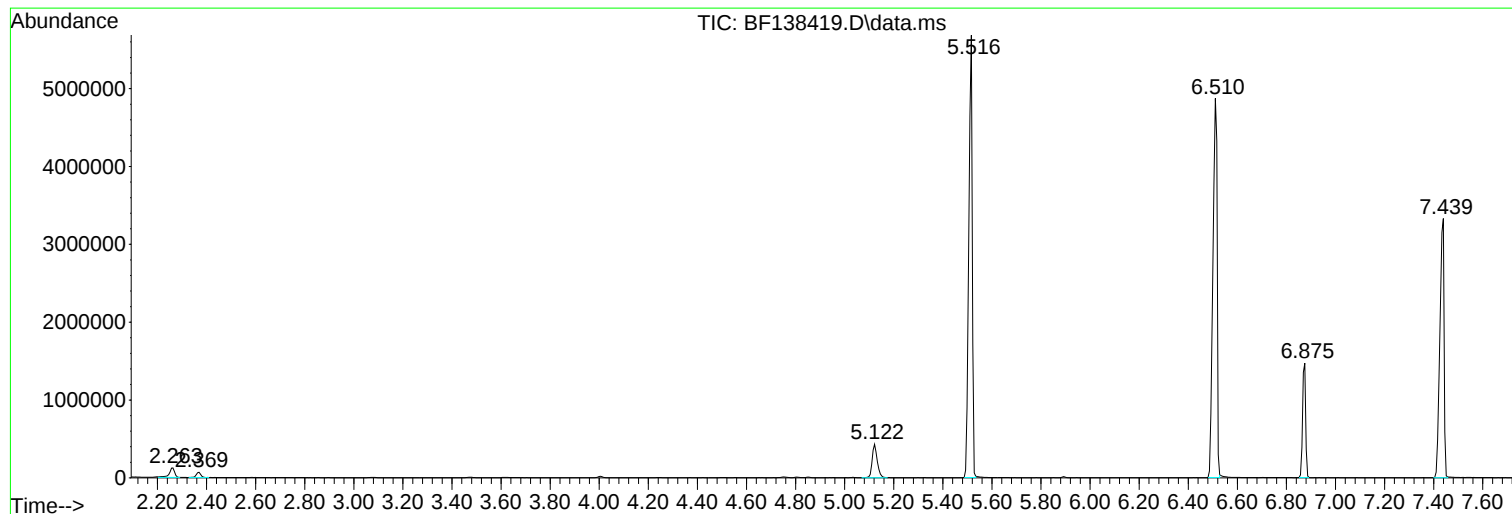
Sum of corrected areas: 40227148

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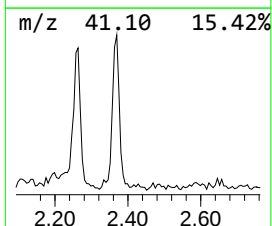
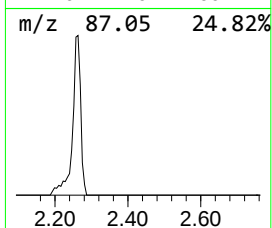
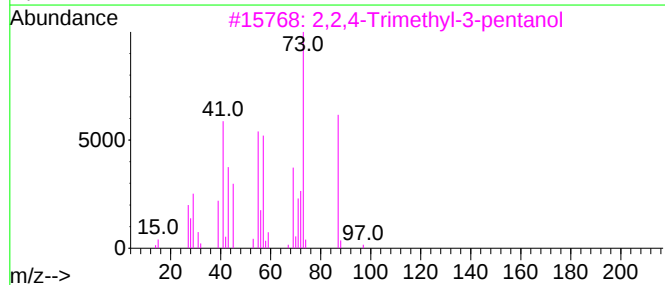
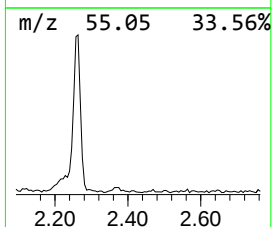
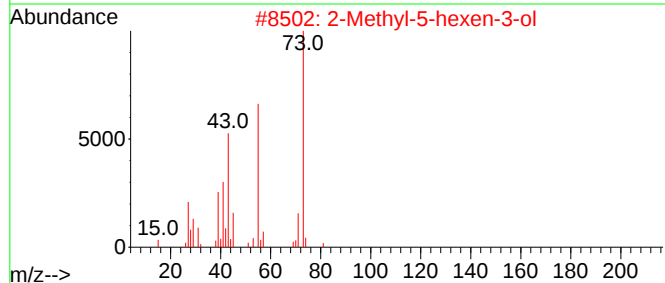
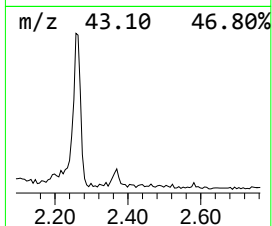
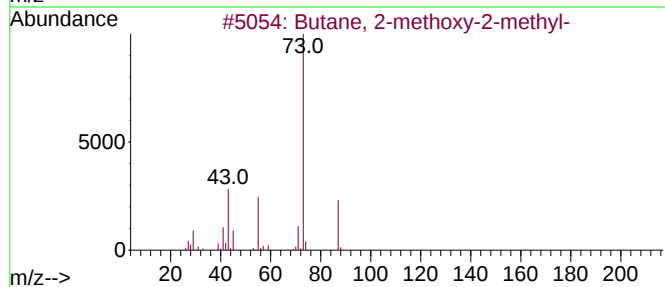
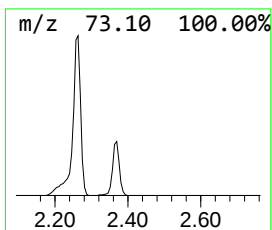
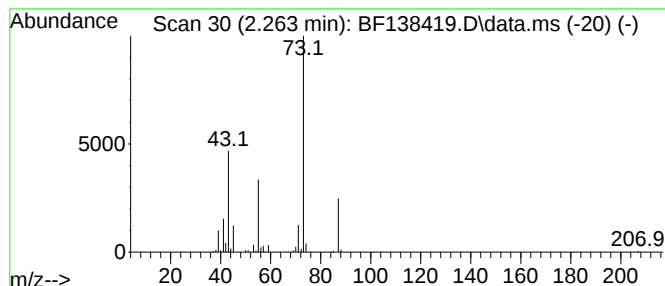
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.263	2.93 ng	187615	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-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	47
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	38
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35



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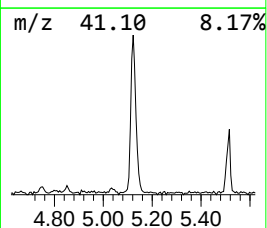
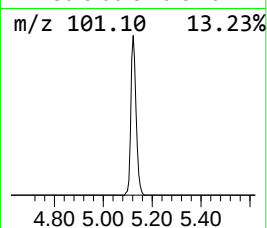
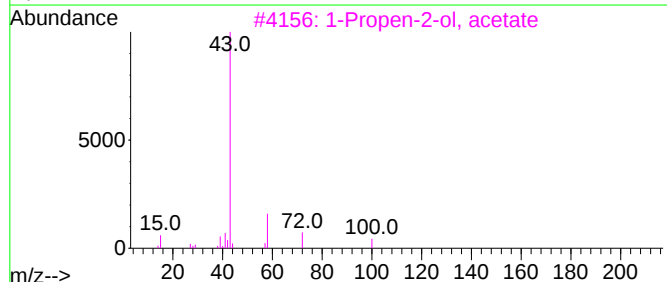
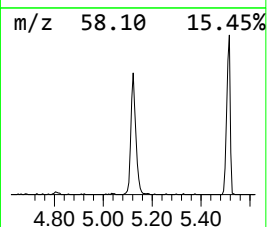
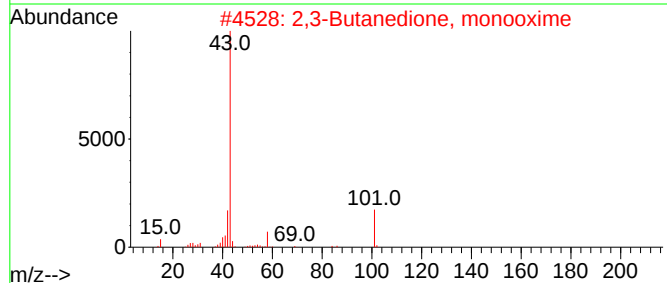
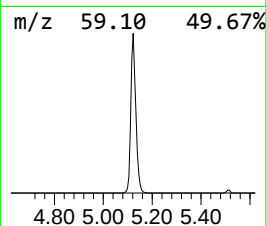
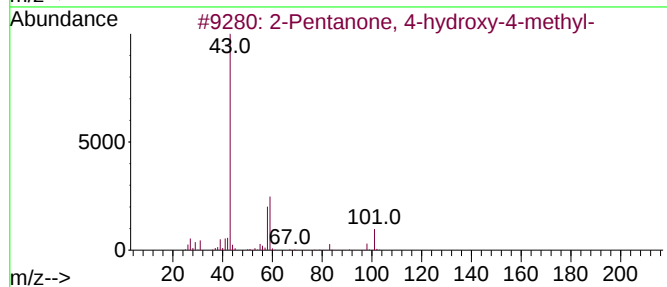
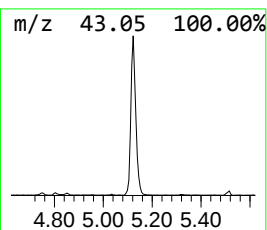
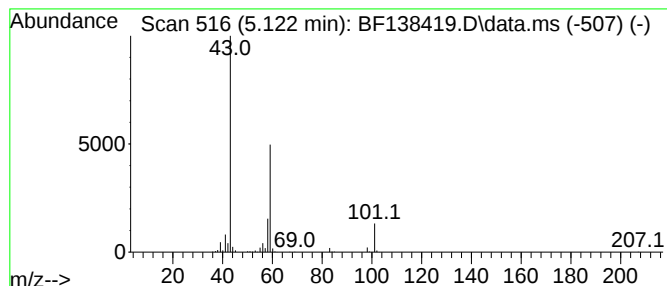
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	9.62 ng	615853	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			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7



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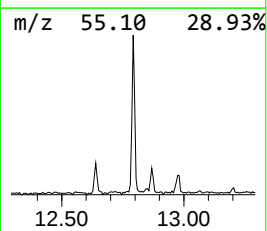
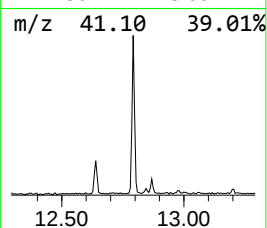
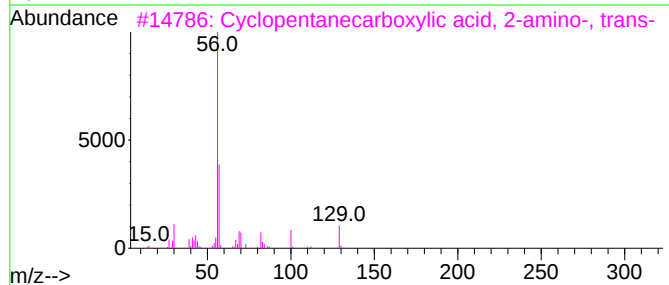
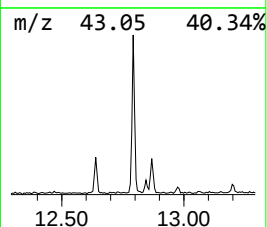
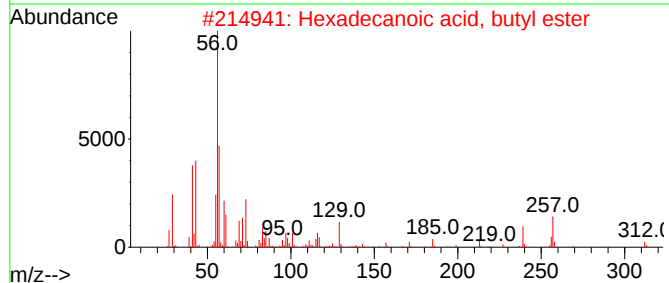
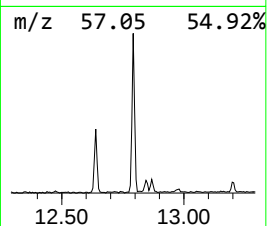
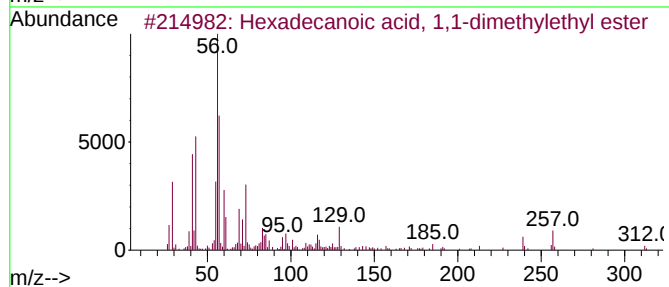
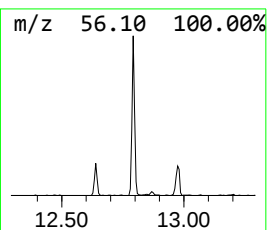
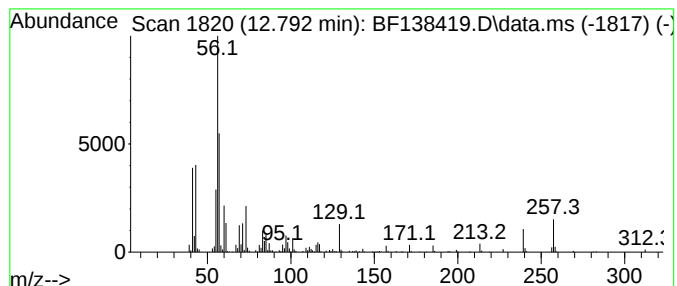
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Peak Number 3 Hexadecanoic acid, 1,1-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.792	6.39 ng	307757	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
4			Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	40
5			Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	35



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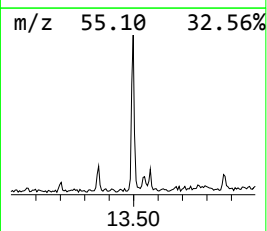
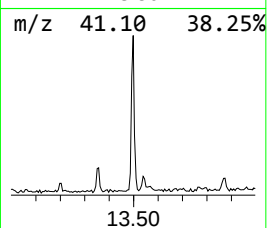
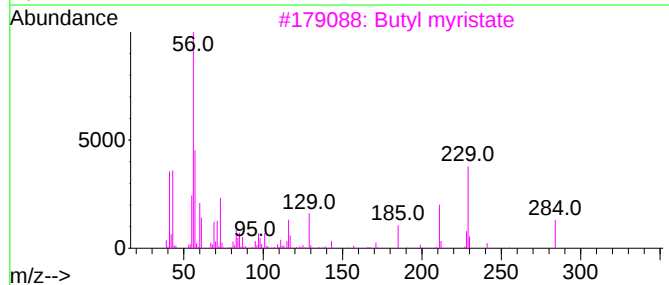
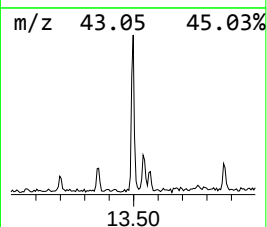
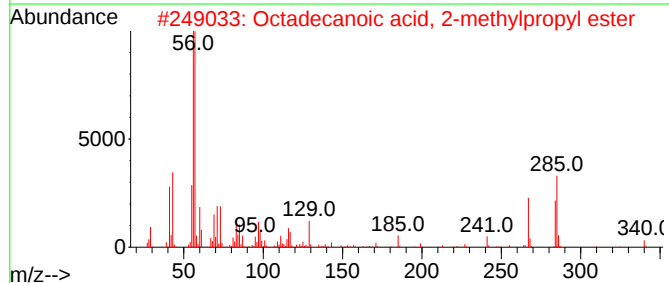
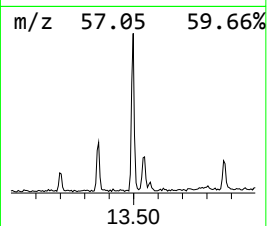
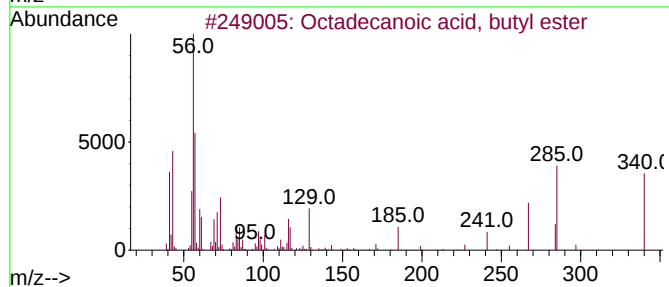
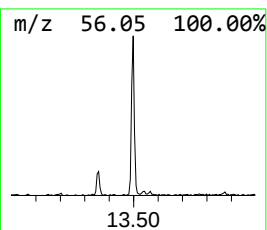
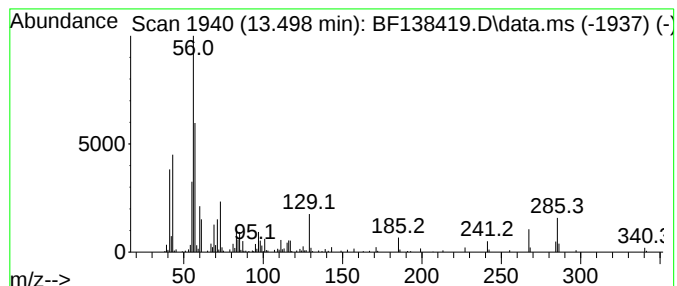
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Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	3.57 ng	172009	Chrysene-d12	14.027

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	70
3			Butyl myristate	284	C18H36O2	000110-36-1	50
4			Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
5			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.263	2.9	ng	187615	1	6.875	1279980	20.0
2-Pentanone, 4-...	5.122	9.6	ng	615853	1	6.875	1279980	20.0
Hexadecanoic ac...	12.792	6.4	ng	307757	5	14.027	963864	20.0
Octadecanoic ac...	13.498	3.6	ng	172009	5	14.027	963864	20.0