

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121823\
 Data File : BG060067.D
 Acq On : 18 Dec 2023 15:31
 Operator : MA/JU
 Sample : 05827-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RT-SB-07-14-15

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_G\Methods\8270-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060067.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.137	3	8	20	rVB	130834	244324	3.79%	1.041%
2	5.529	406	415	427	rBV	921774	1534008	23.78%	6.538%
3	7.109	677	684	694	rBV	984393	1684799	26.12%	7.180%
4	7.955	821	828	836	rVB2	210341	360208	5.58%	1.535%
5	9.119	1018	1026	1034	rVB	552970	991570	15.37%	4.226%
6	10.758	1297	1305	1313	rBV	270427	477048	7.40%	2.033%
7	13.220	1717	1724	1730	rVB	1825175	2847430	44.14%	12.135%
8	14.595	1952	1958	1965	rVB	532889	791722	12.27%	3.374%
9	15.164	2048	2055	2068	rBV4	33895	122077	1.89%	0.520%
10	16.081	2204	2211	2223	rBV	2159700	3126748	48.47%	13.326%
11	17.344	2419	2426	2432	rBV	828453	1202659	18.65%	5.126%
12	18.231	2572	2577	2586	rBV	267139	363667	5.64%	1.550%
13	19.506	2791	2794	2799	rBV6	82521	108010	1.67%	0.460%
14	19.965	2866	2872	2878	rBV	5119688	6450255	100.00%	27.490%
15	21.263	3090	3093	3098	rVB3	155141	224147	3.48%	0.955%
16	21.616	3147	3153	3159	rVB	951947	1485445	23.03%	6.331%
17	24.806	3689	3696	3708	rVB2	510153	1450061	22.48%	6.180%

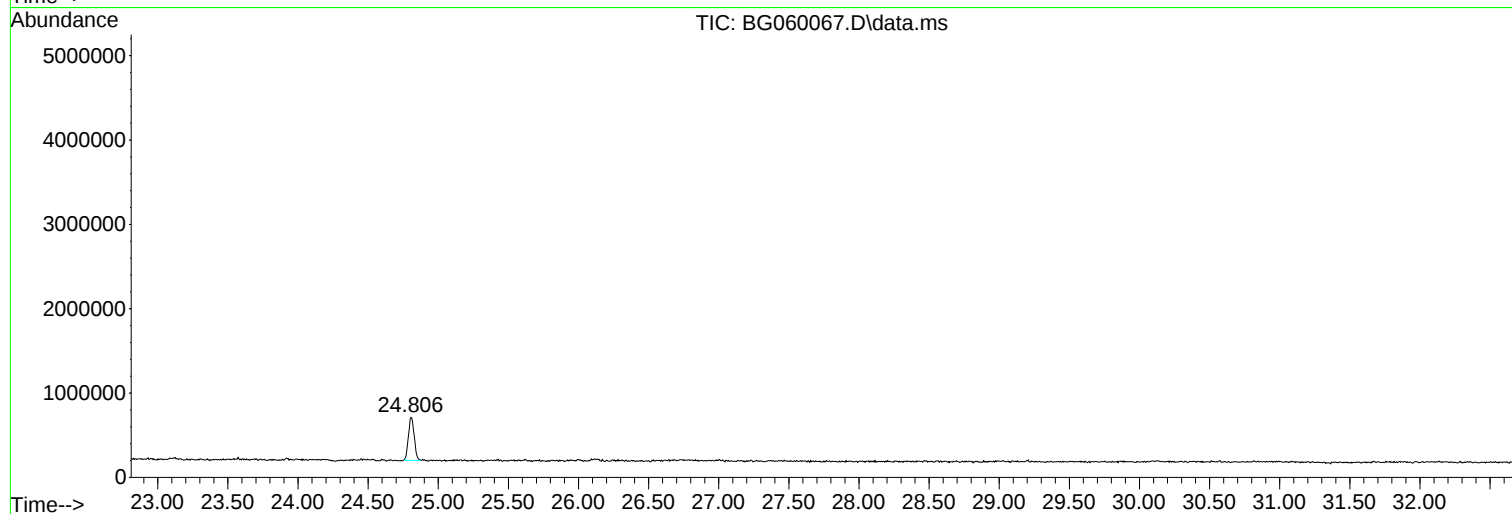
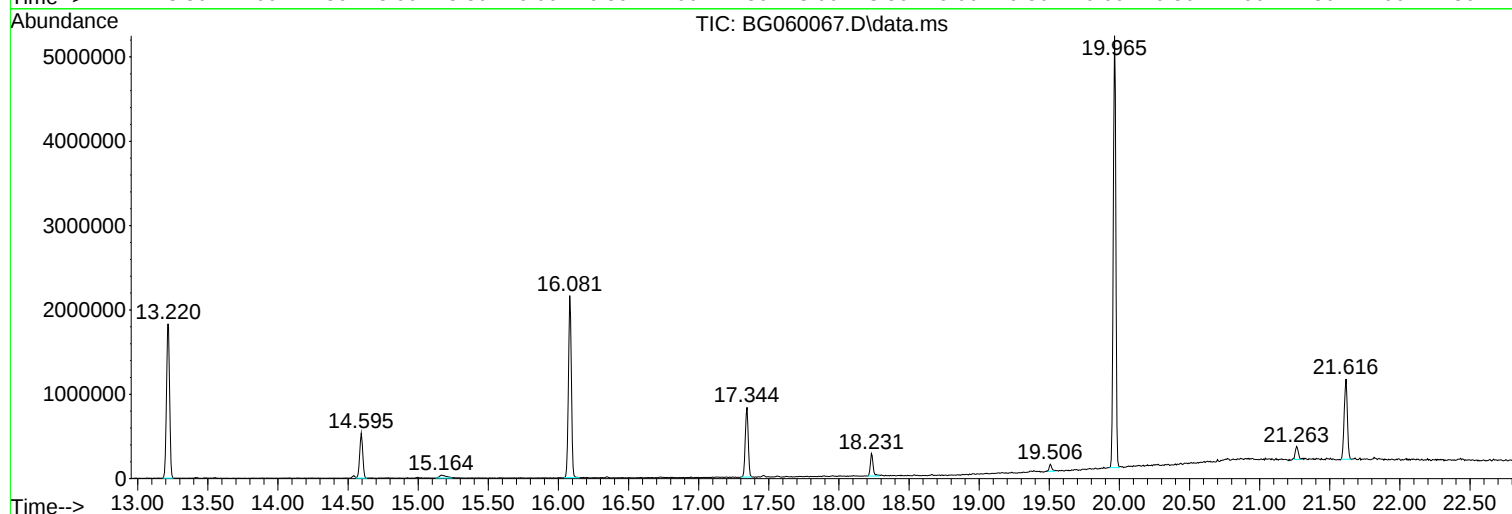
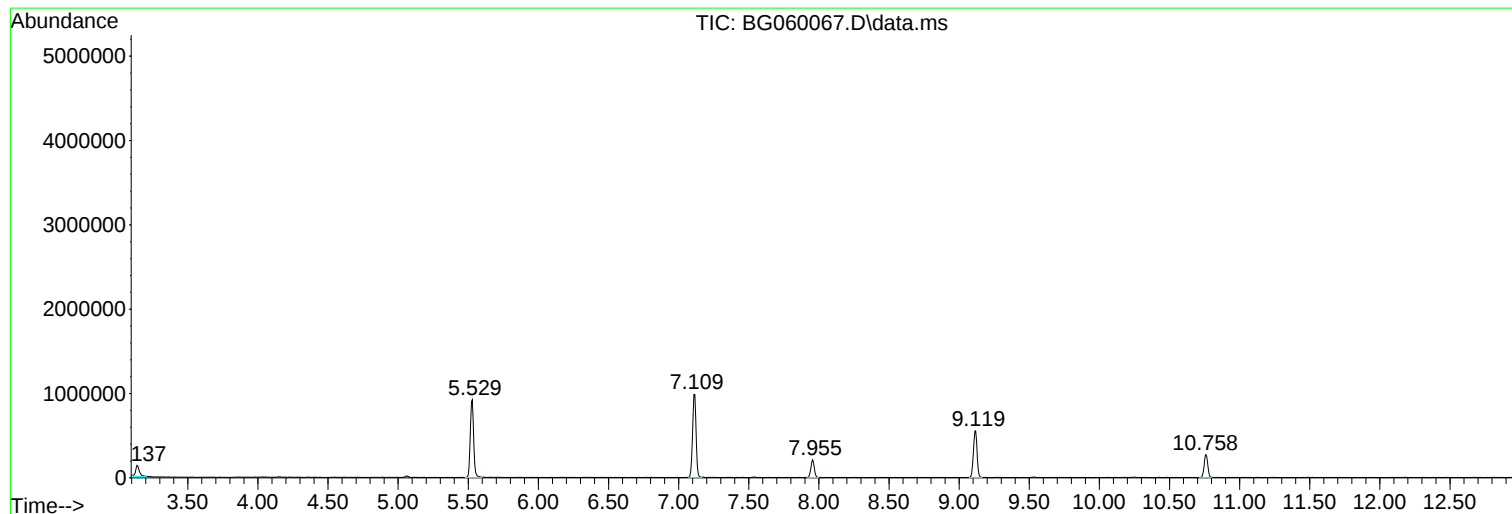
Sum of corrected areas: 23464178

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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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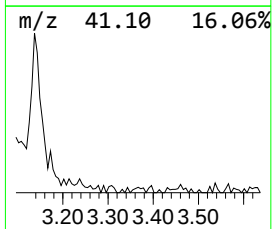
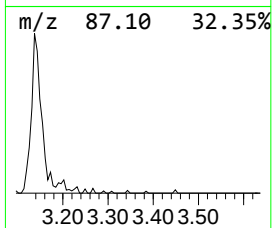
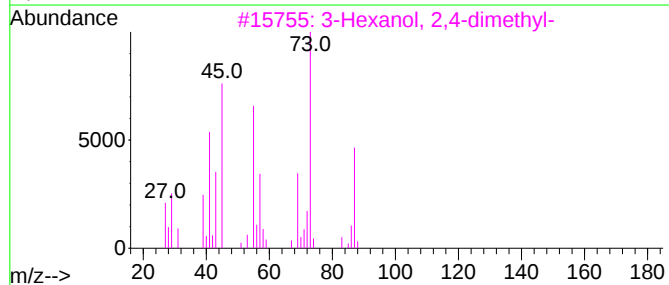
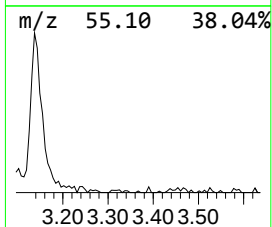
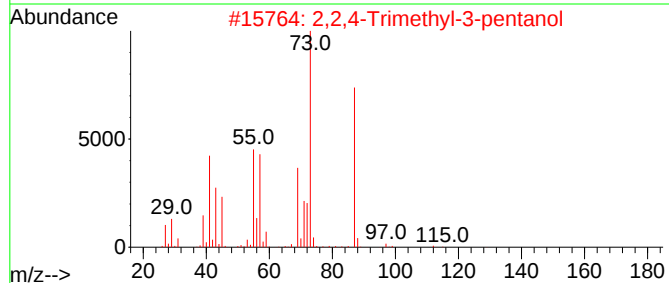
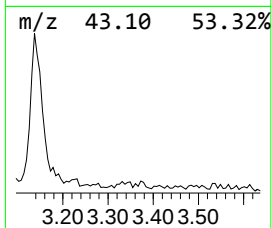
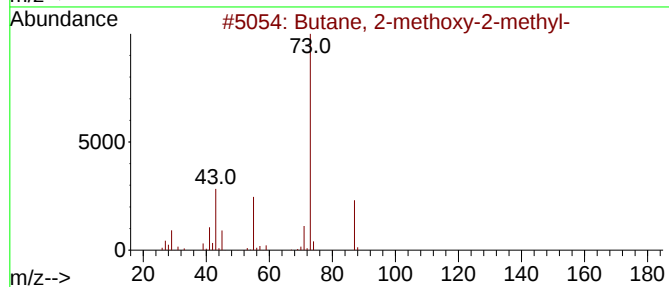
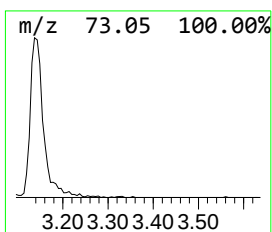
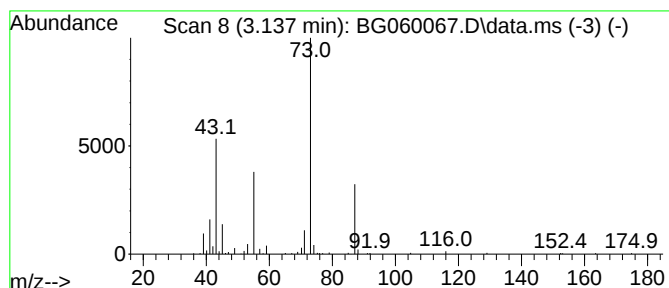
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.137	13.57 ng	244324	1,4-Dichlorobenzene-d4	7.955

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	42
3			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	38
4			Butanoic acid, 2-hydroxy-2-methyl-	132	C6H12O3	032793-34-3	37
5			Myo-Inositol, 4-C-methyl-	194	C7H14O6	000472-95-7	33



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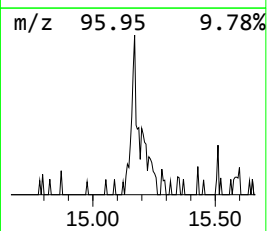
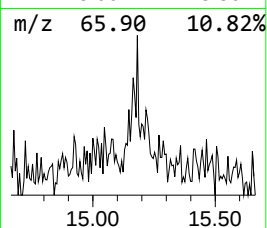
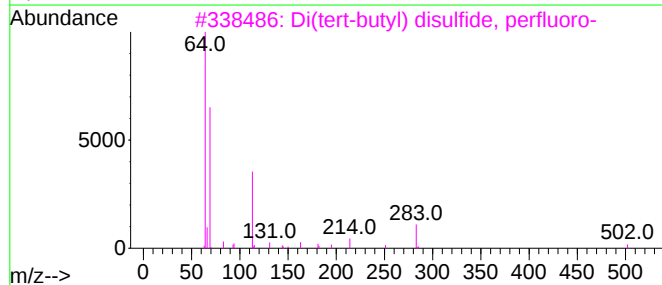
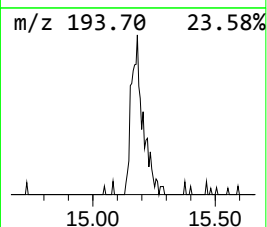
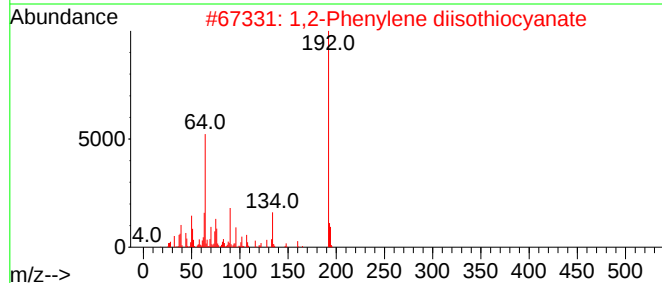
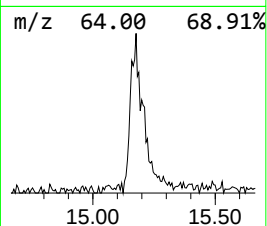
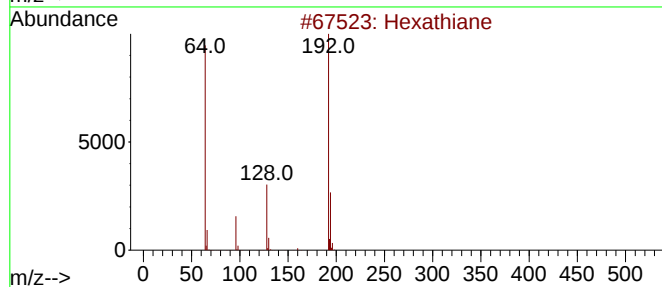
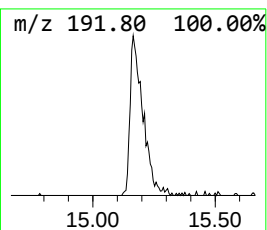
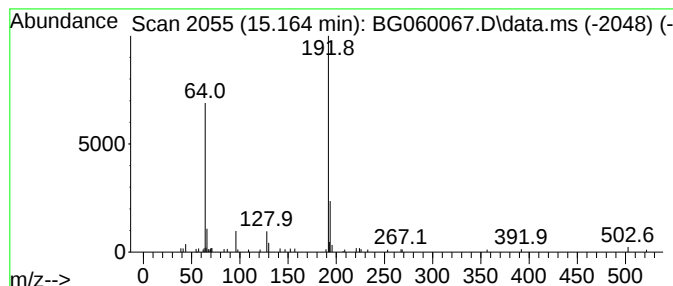
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexathiane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.165	3.08 ng	122077	Acenaphthene-d10	14.595

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiane	192	S6	013798-23-7	91
2			1,2-Phenylene diisothiocyanate	192	C8H4N2S2	071105-17-4	40
3			Di(tert-butyl) disulfide, perflu...	502	C8F18S2	034880-30-3	37
4			Cyclic octaatomic sulfur	256	S8	010544-50-0	33
5			2-Chloro-1-(5-chloro-2-methyl-1H...	241	C11H9Cl2NO	620603-92-1	12



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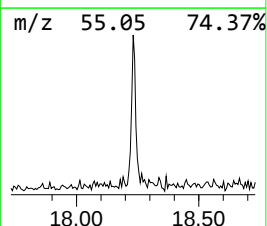
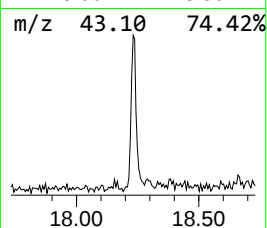
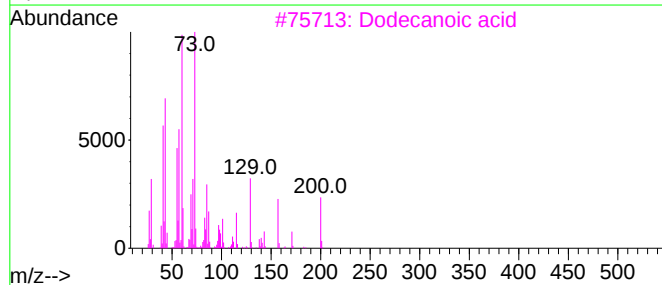
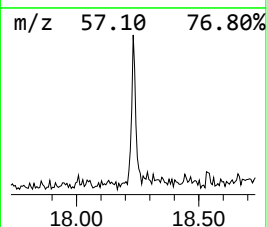
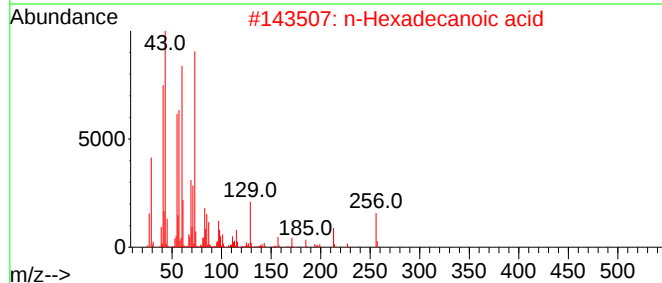
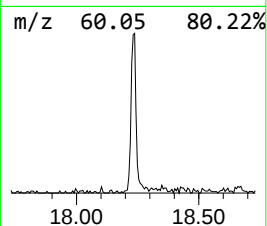
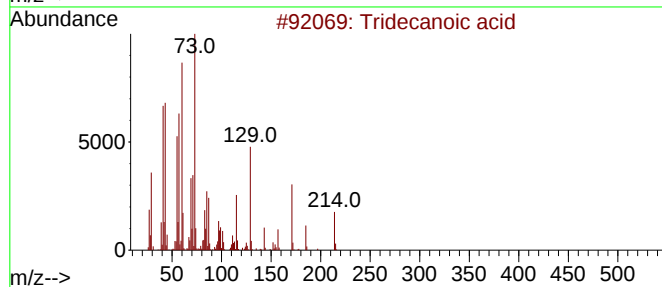
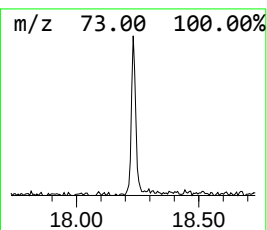
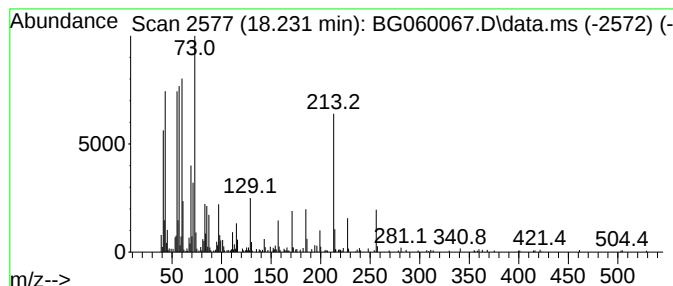
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Peak Number 3 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.232	6.05 ng	363667	Phenanthrene-d10	17.344

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	90
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3			Dodecanoic acid	200	C12H24O2	000143-07-7	49
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	43



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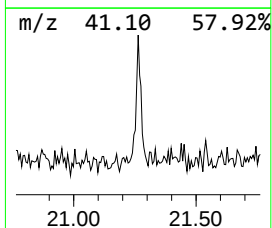
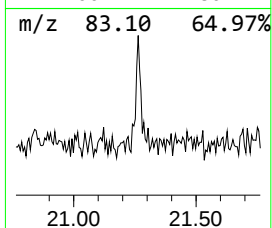
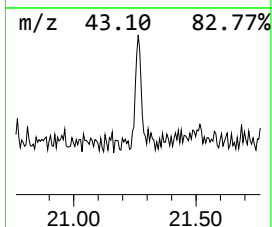
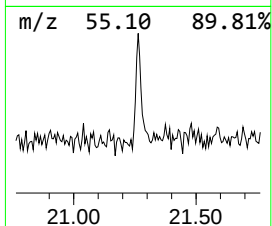
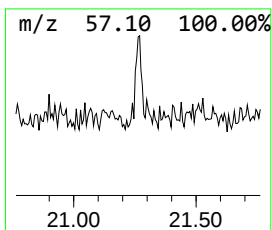
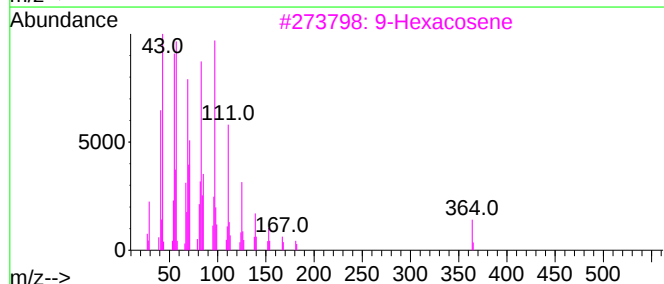
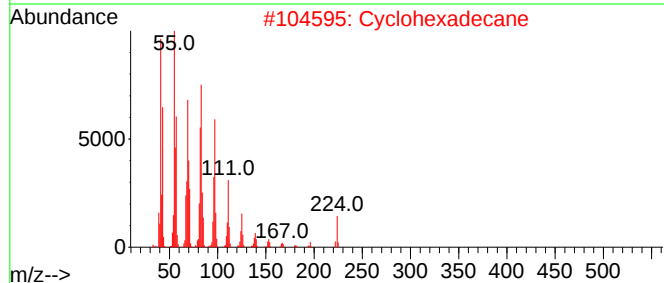
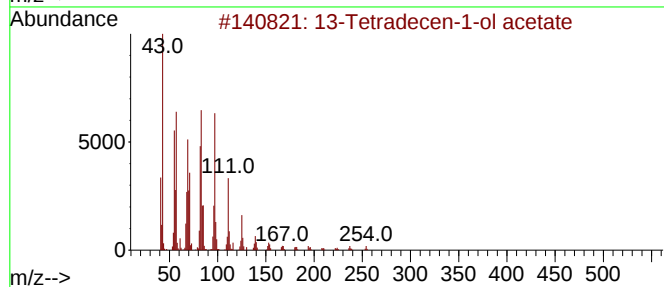
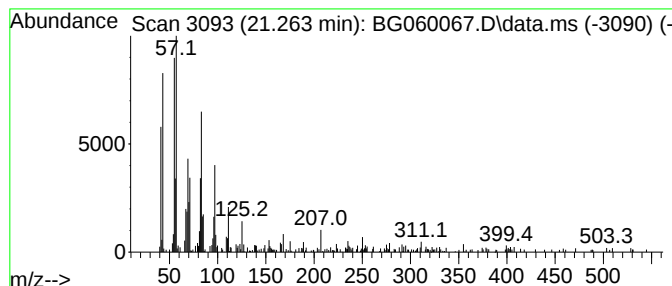
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Peak Number 4 13-Tetradecen-1-ol acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.263	3.02 ng	224147	Chrysene-d12	21.616	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	96
2	Cyclohexadecane	224	C16H32	000295-65-8	95
3	9-Hexacosene	364	C26H52	071502-22-2	93
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
5	1-Hexacosene	364	C26H52	018835-33-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.137	13.6	ng	244324	1	7.955	360208	20.0
Hexathiane	15.165	3.1	ng	122077	3	14.595	791722	20.0
Tridecanoic acid	18.232	6.0	ng	363667	4	17.344	1202660	20.0
13-Tetradecen-1...	21.263	3.0	ng	224147	5	21.616	1485450	20.0