

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061917\
 Data File : BF096002.D
 Acq On : 19 Jun 2017 12:57
 Operator : SJ/MA
 Sample : PB99843BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB99843BL

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:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.557	10	12	65	rVB	1586295	3544280	100.00%	16.087%
2	4.516	511	515	535	rBV	57203	196047	5.53%	0.890%
3	5.198	627	631	659	rBV	962933	1926070	54.34%	8.742%
4	6.875	911	916	927	rBV	1129428	1779855	50.22%	8.079%
5	6.963	927	931	950	rVB	1439144	2222051	62.69%	10.086%
6	7.304	985	989	1003	rBV	290211	417276	11.77%	1.894%
7	7.539	1024	1029	1045	rBV	1135866	1592078	44.92%	7.226%
8	8.228	1141	1146	1174	rBV	736813	1211497	34.18%	5.499%
9	9.333	1330	1334	1350	rBV	368923	580291	16.37%	2.634%
10	11.116	1630	1637	1654	rBV	1789441	2486171	70.15%	11.285%
11	12.157	1809	1814	1829	rBV2	468020	656241	18.52%	2.979%
12	13.451	2029	2034	2060	rBV	825961	1223726	34.53%	5.554%
13	14.551	2216	2221	2236	rBV	420033	639642	18.05%	2.903%
14	16.792	2597	2602	2606	rBV	231522	247841	6.99%	1.125%
15	16.898	2617	2620	2621	rBV	37686	36418	1.03%	0.165%
16	16.933	2621	2626	2636	rVB2	1780732	2247820	63.42%	10.203%
17	17.721	2755	2760	2765	rBV	156853	172310	4.86%	0.782%
18	18.274	2851	2854	2871	rVV	346098	496063	14.00%	2.252%
19	19.950	3135	3139	3152	rBV	221057	355852	10.04%	1.615%

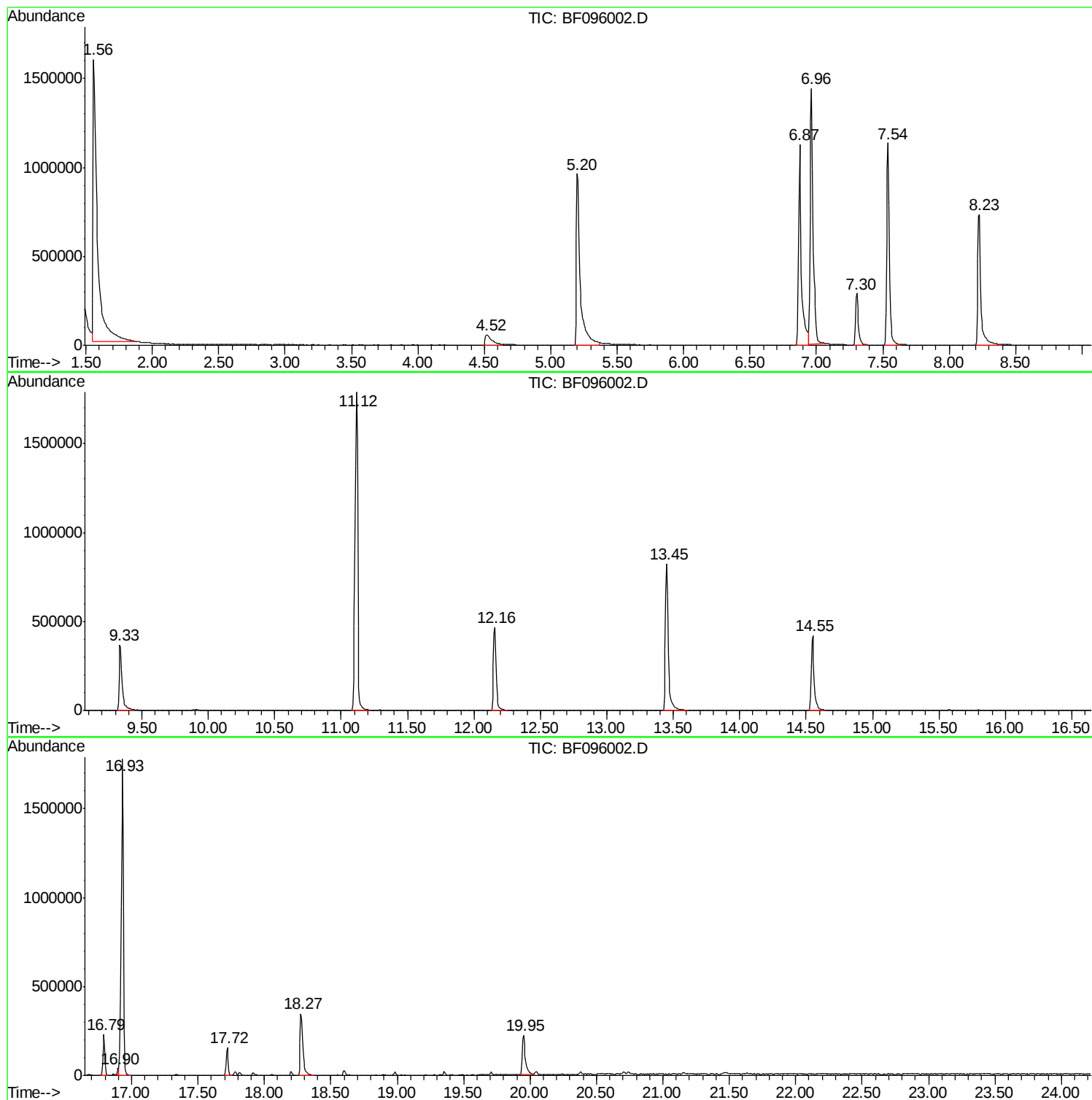
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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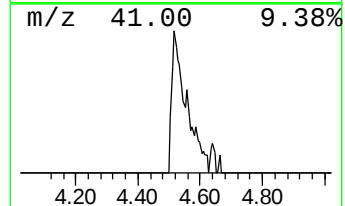
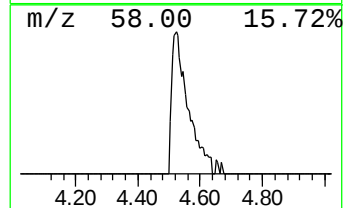
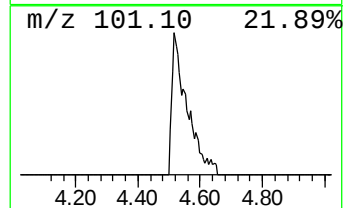
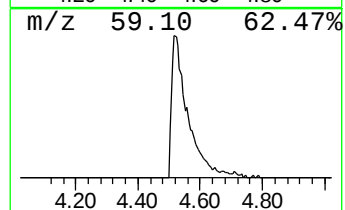
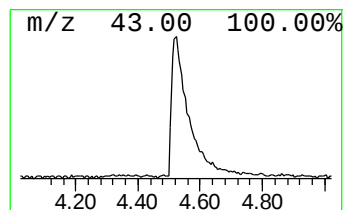
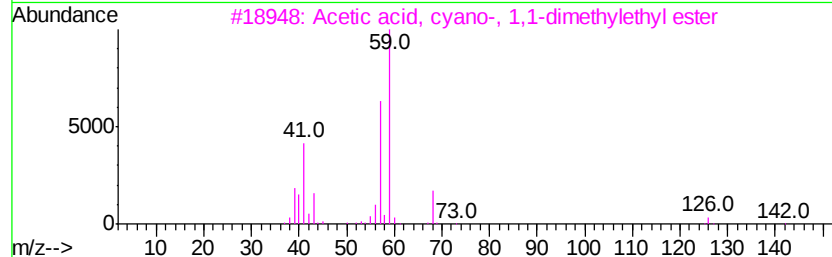
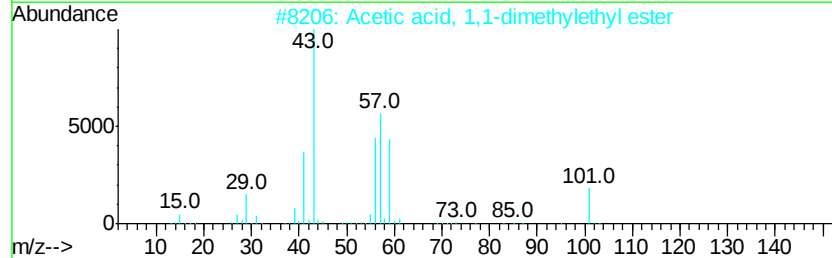
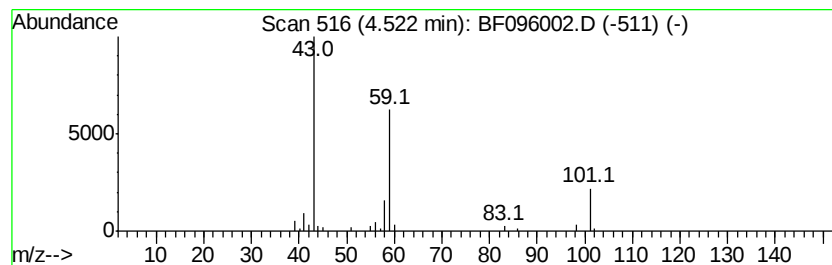
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	9.40 ng	196047	1,4-Dichlorobenzene-d4	7.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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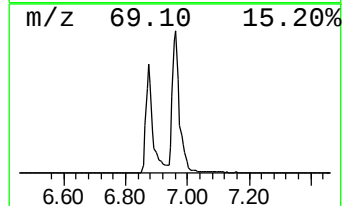
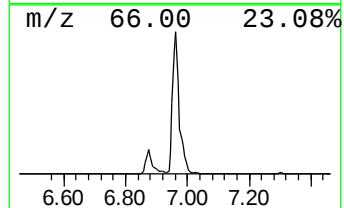
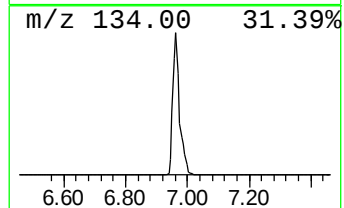
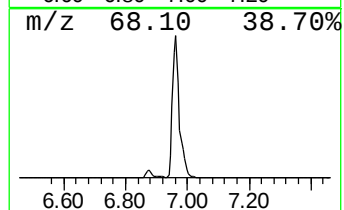
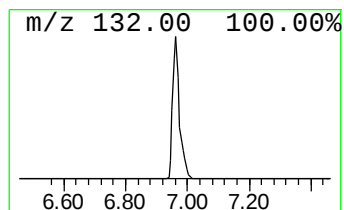
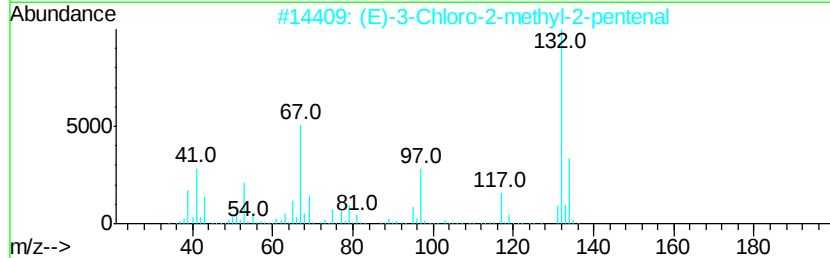
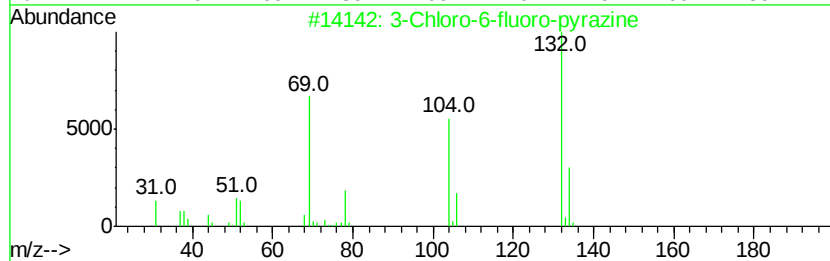
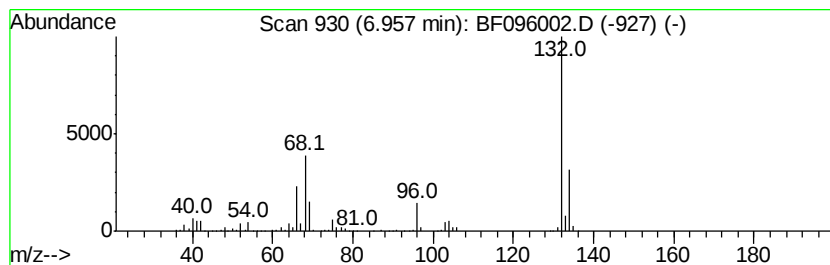
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Peak Number 3 unknown6.96 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	106.50 ng	2222050	1,4-Dichlorobenzene-d4	7.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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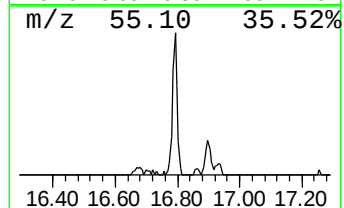
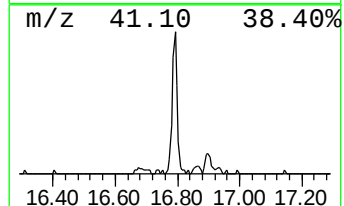
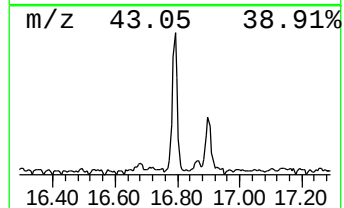
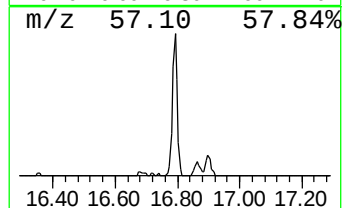
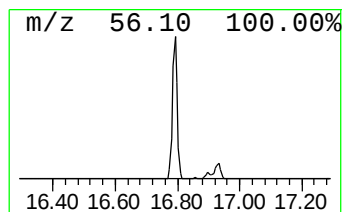
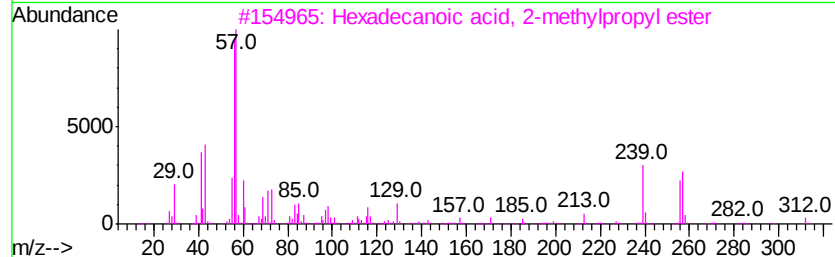
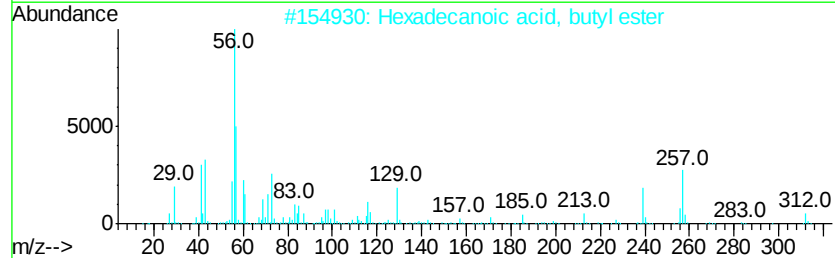
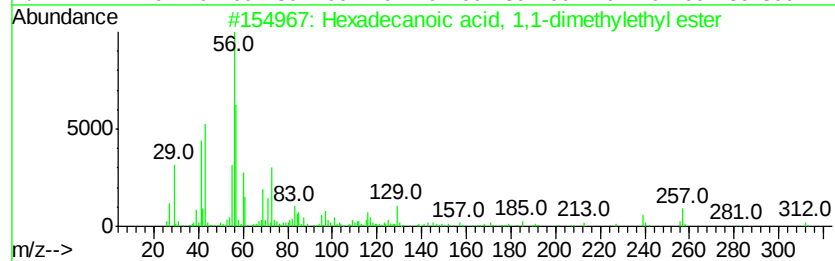
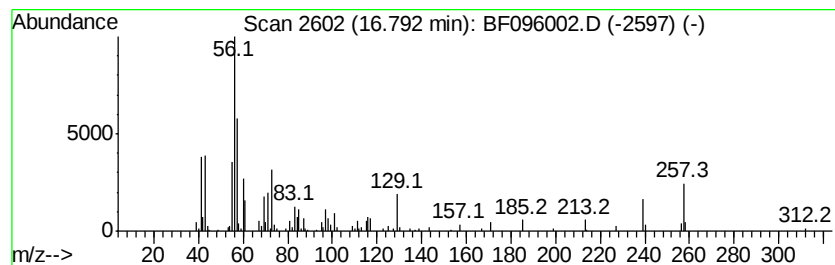
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.79	9.99 ng	247841	Chrysene-d12	18.27

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	90
3			Hexadecanoic acid, 2-methylpropv...	312	C20H40O2	000110-34-9	64
4			Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	42
5			2-Methyl-1-octadecene	266	C19H38	061868-20-0	35



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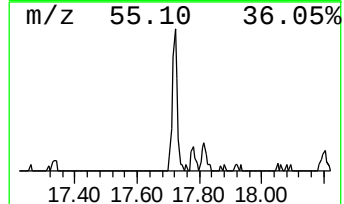
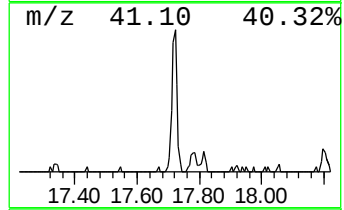
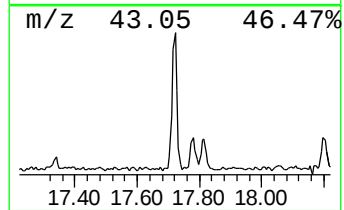
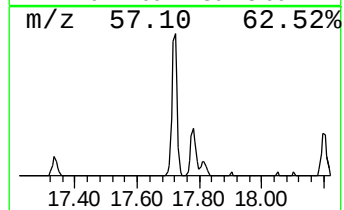
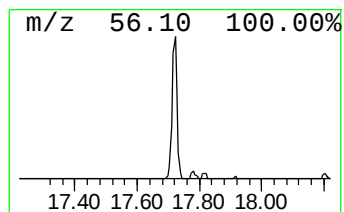
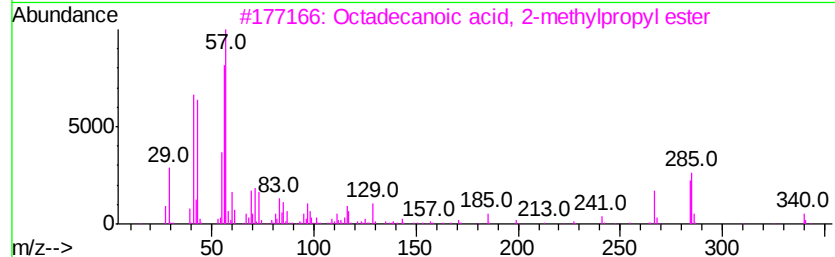
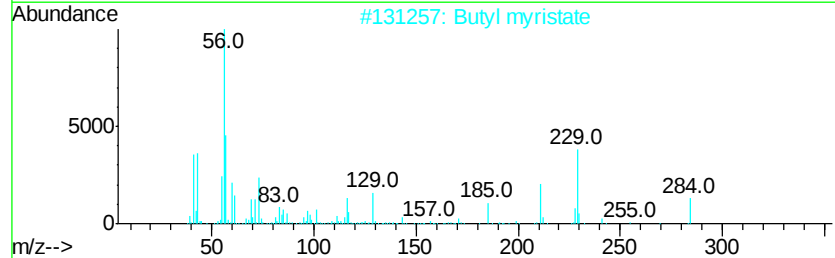
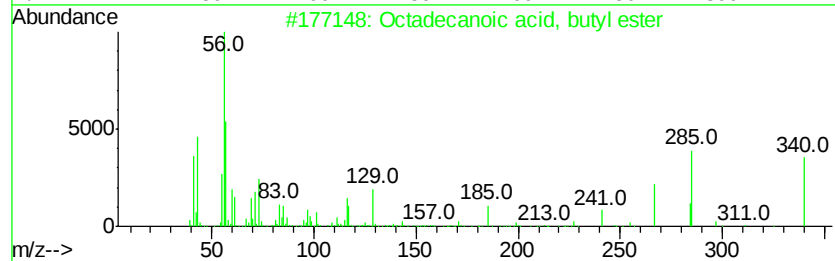
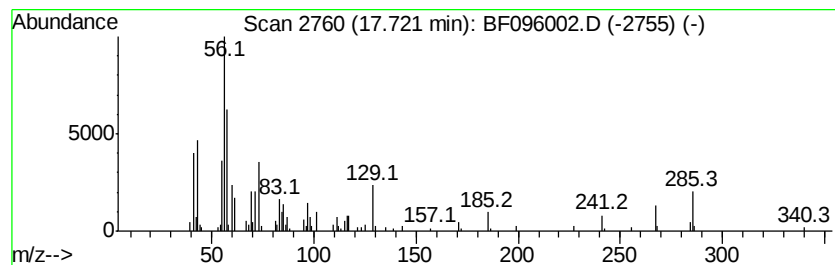
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Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.72	6.95 ng	172310	Chrysene-d12	18.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Butyl myristate	284	C18H36O2	000110-36-1	59
3		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	50
4		7-Heptadecanol, 7-methyl-	270	C18H38O	055723-93-8	32
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.52	9.4	ng	196047	1	7.30	417276	20.0
unknown6.96	6.96	106.5	ng	2222050	1	7.30	417276	20.0
Hexadecanoic acid...	16.79	10.0	ng	247841	5	18.27	496063	20.0
Octadecanoic acid...	17.72	7.0	ng	172310	5	18.27	496063	20.0