

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072321\
 Data File : BF124718.D
 Acq On : 23 Jul 2021 17:58
 Operator : JU/CG
 Sample : M3152-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VAULT-B

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-BF072221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124718.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	12	16	19	rBB	9878	11140	5.77%	0.864%
2	5.093	508	511	515	rBB	3196	3543	1.84%	0.275%
3	5.487	573	578	581	rBB	152996	142030	73.63%	11.019%
4	6.493	743	749	752	rBB	142400	145924	75.65%	11.322%
5	6.869	810	813	816	rBB	49246	36144	18.74%	2.804%
6	7.428	904	908	911	rBB	98589	96994	50.28%	7.525%
7	8.051	1011	1014	1017	rBV	47467	34076	17.66%	2.644%
8	8.151	1027	1031	1034	rBB	62292	51359	26.62%	3.985%
9	9.228	1209	1214	1217	rBB	231160	191128	99.08%	14.829%
10	9.904	1326	1329	1332	rBB	71519	59850	31.03%	4.643%
11	10.692	1459	1463	1466	rBB	126538	120040	62.23%	9.313%
12	11.392	1578	1582	1585	rBB	80552	60269	31.24%	4.676%
13	11.916	1666	1671	1674	rBB	33693	28672	14.86%	2.225%
14	12.704	1800	1805	1808	rBB	19668	18197	9.43%	1.412%
15	12.980	1848	1852	1855	rBB	225621	192902	100.00%	14.966%
16	13.874	2000	2004	2011	rBB2	8128	11708	6.07%	0.908%
17	14.027	2027	2030	2033	rBB	53666	44961	23.31%	3.488%
18	14.192	2056	2058	2060	rBB	4631	2851	1.48%	0.221%
19	14.498	2107	2110	2112	rBB	3706	2829	1.47%	0.219%
20	15.498	2276	2280	2284	rBV2	28487	34290	17.78%	2.660%

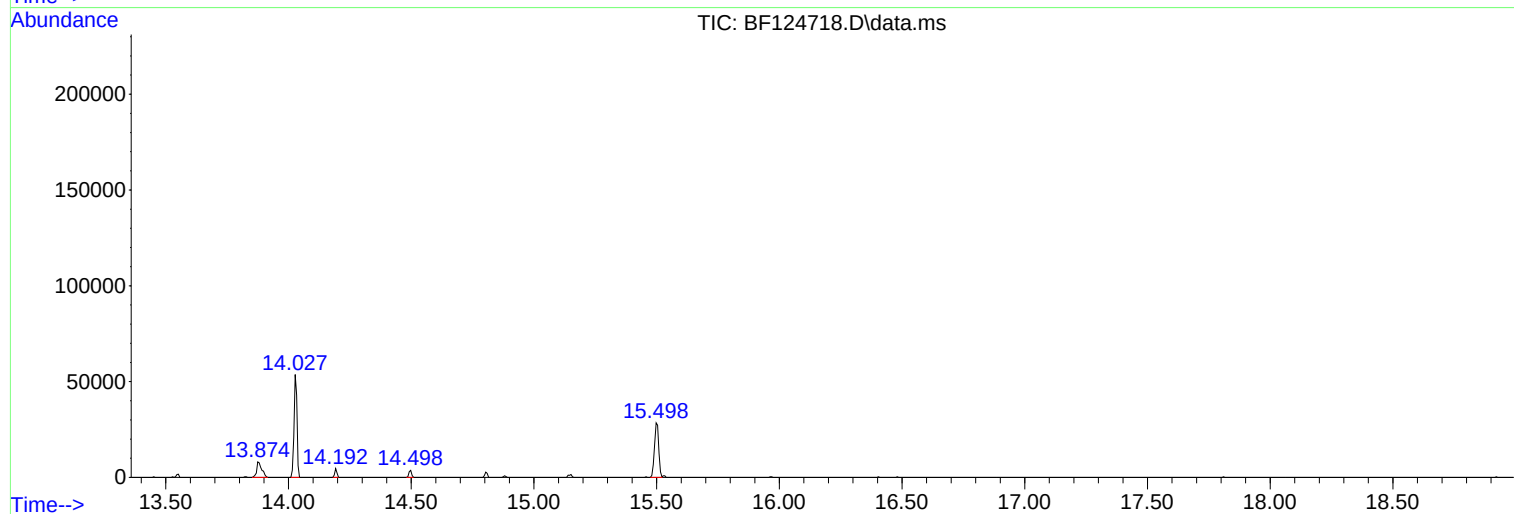
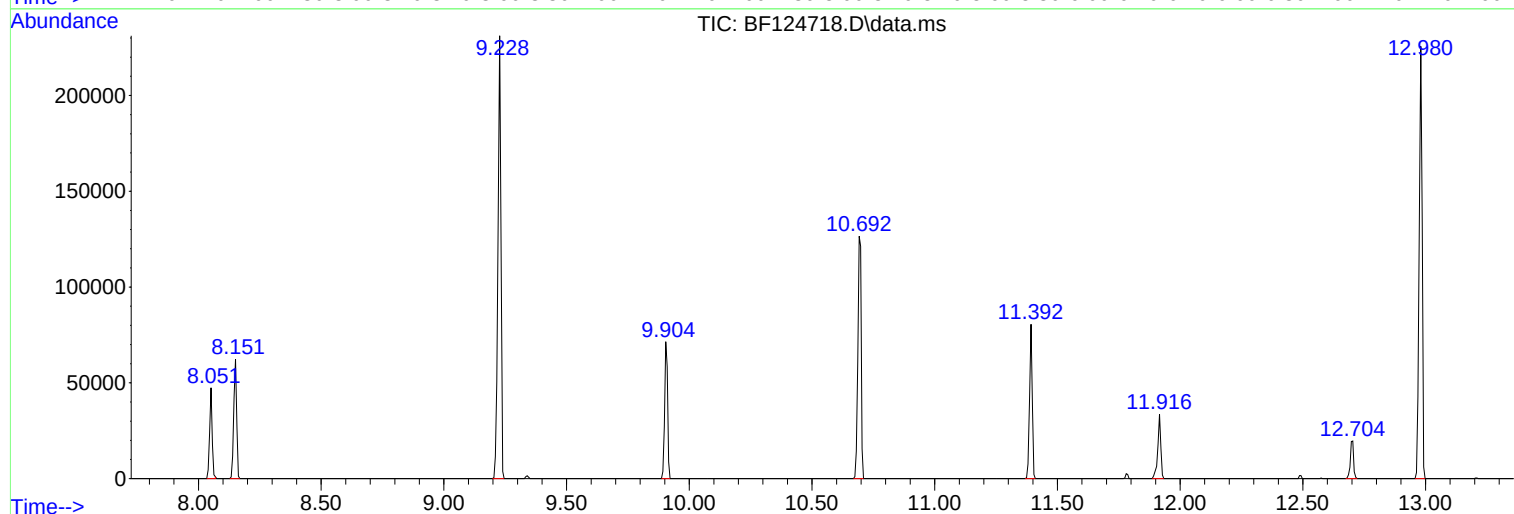
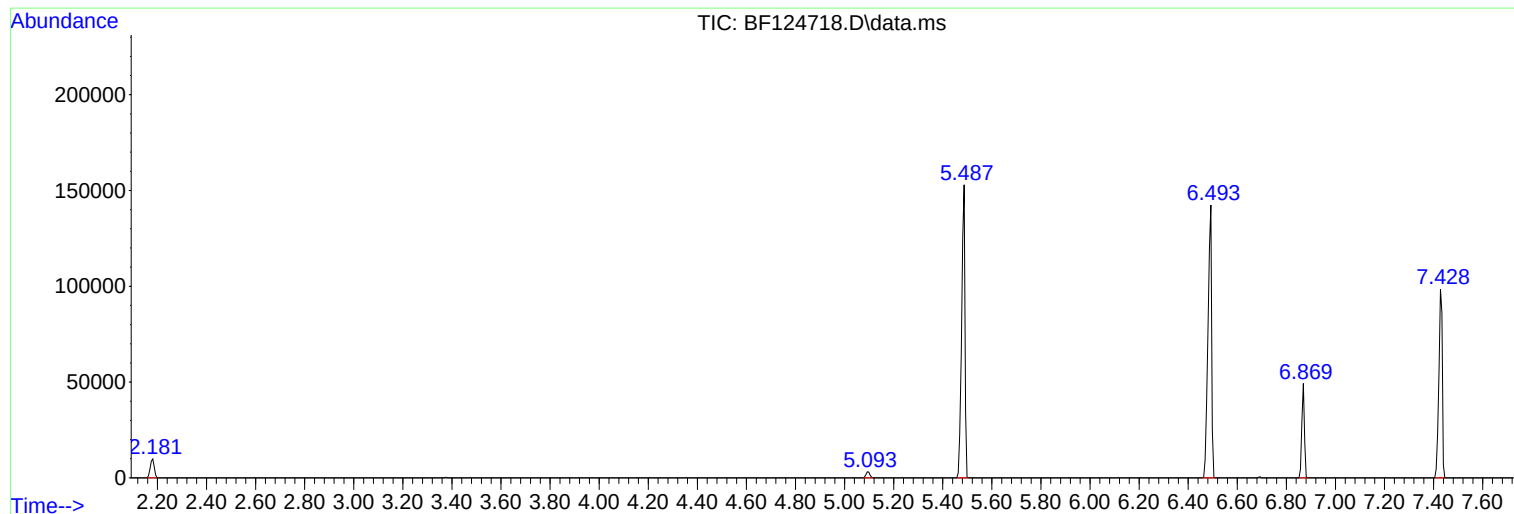
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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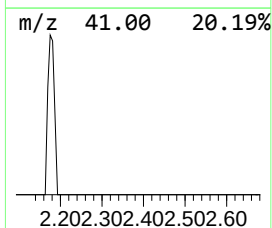
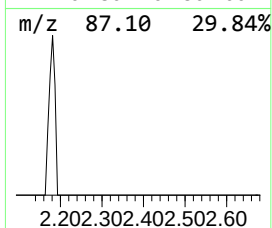
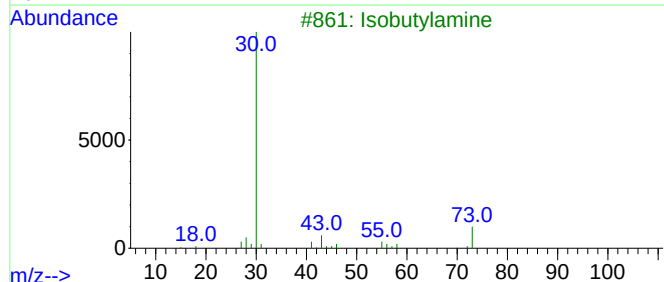
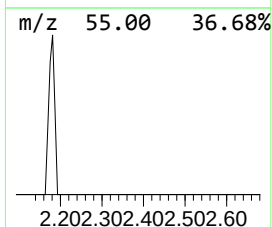
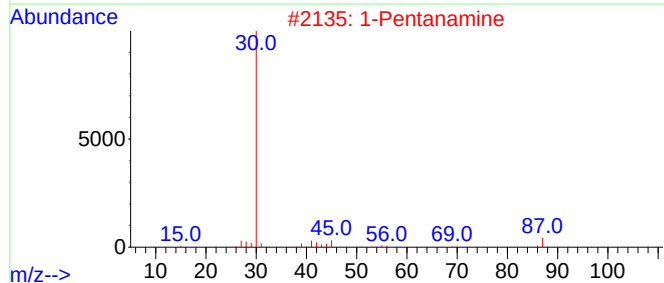
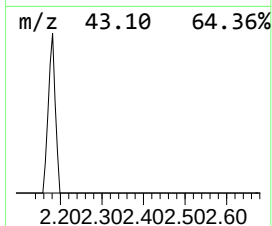
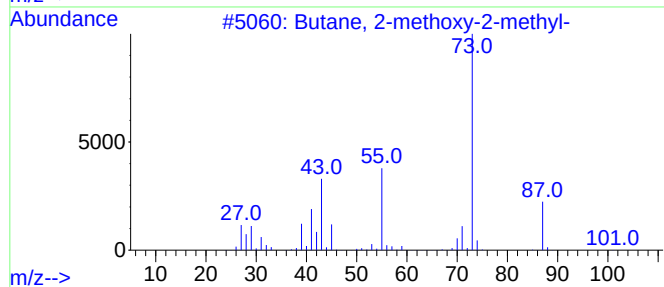
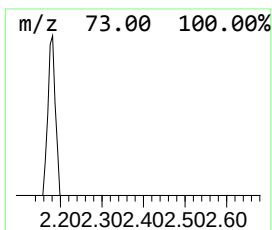
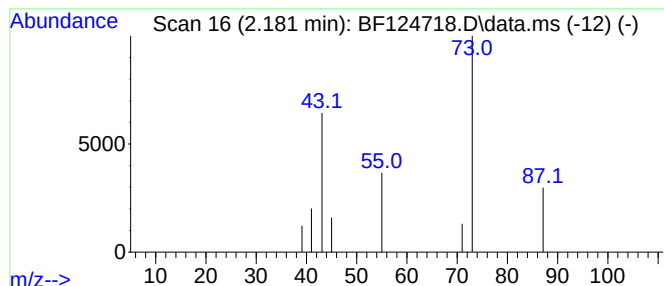
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	6.16 ng	11140	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	64
2			1-Pentanamine	87	C5H13N	000110-58-7	4
3			Isobutylamine	73	C4H11N	000078-81-9	4
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	4
5			2-Pentanol, acetate	130	C7H14O2	000626-38-0	4



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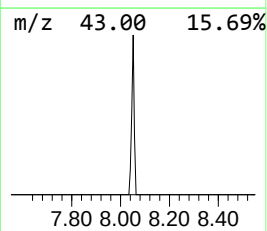
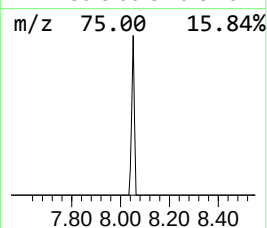
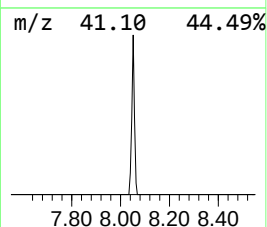
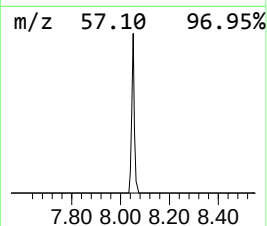
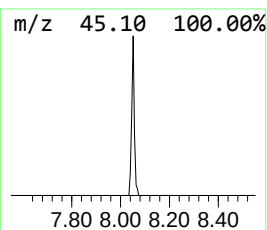
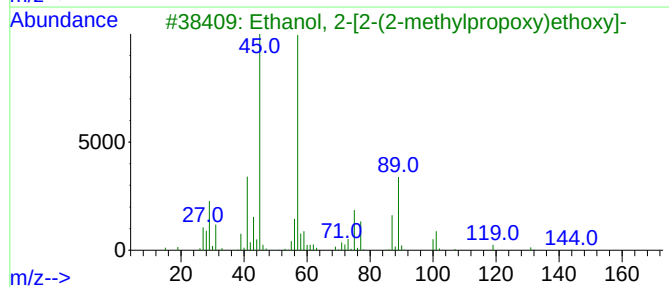
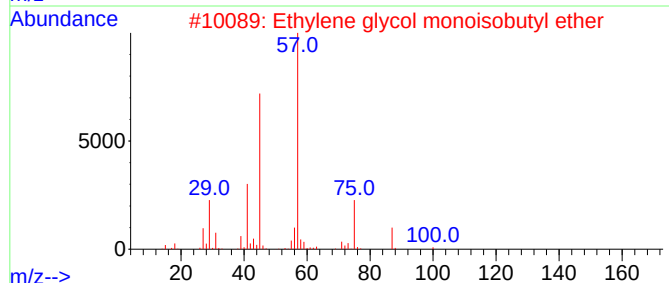
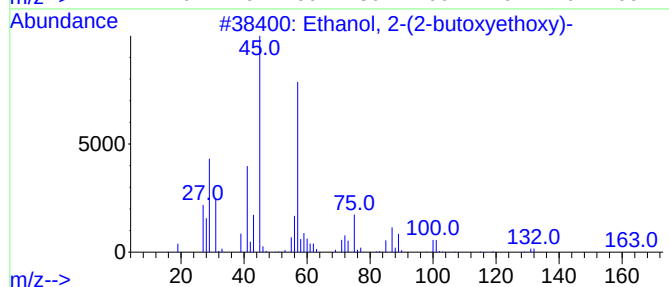
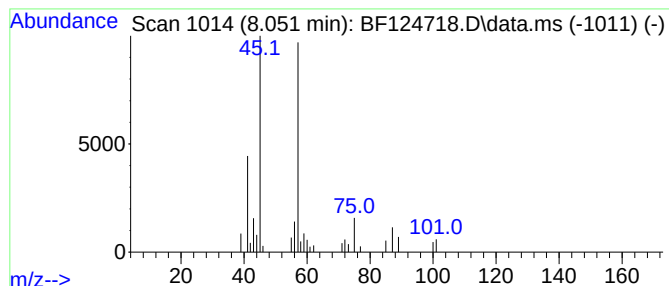
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	13.27 ng	34076	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	50
5			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47



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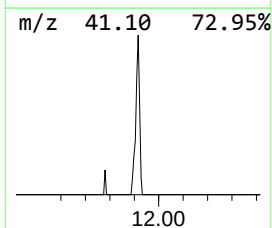
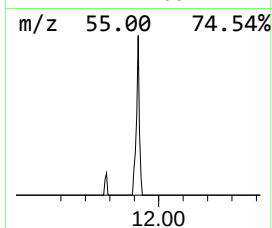
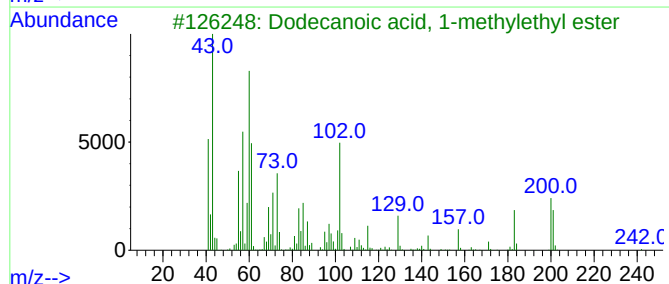
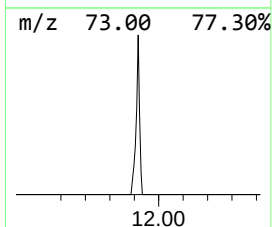
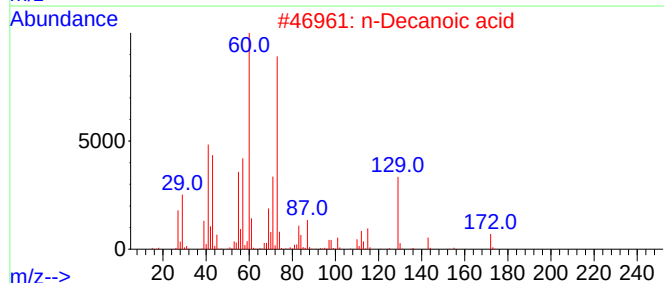
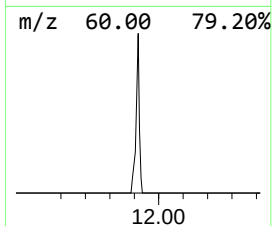
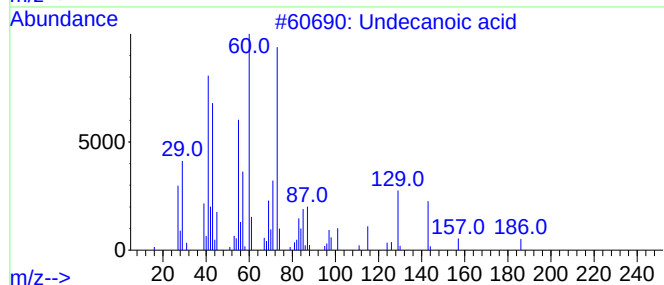
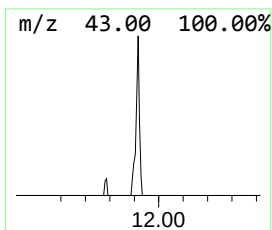
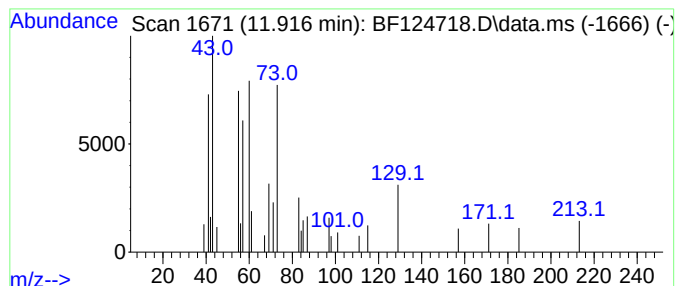
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Peak Number 3 Undecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	9.51 ng	28672	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	59
2			n-Decanoic acid	172	C10H20O2	000334-48-5	53
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	50
4			Heptanoic acid	130	C7H14O2	000111-14-8	47
5			Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	47



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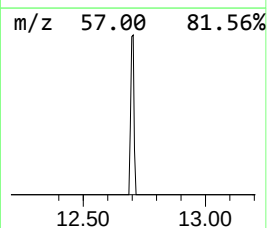
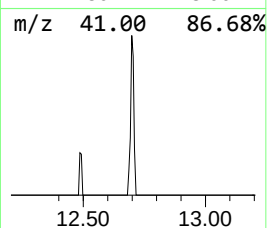
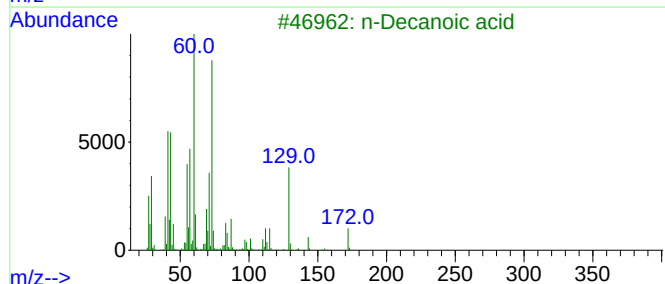
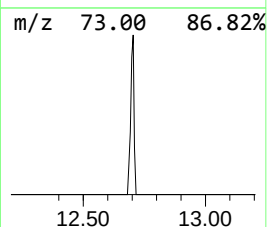
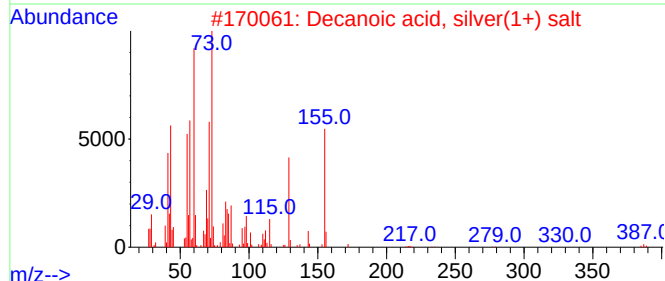
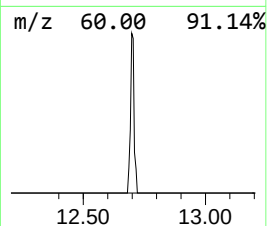
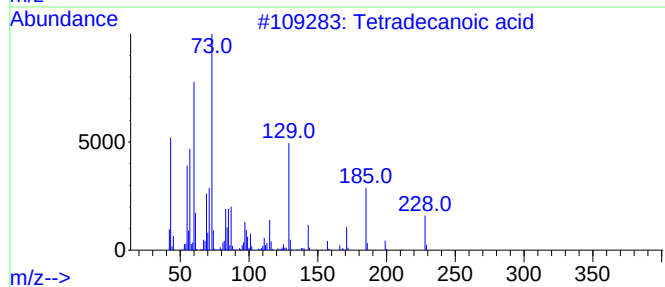
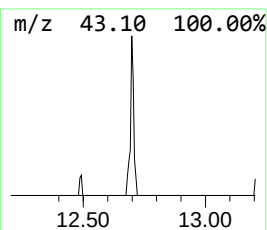
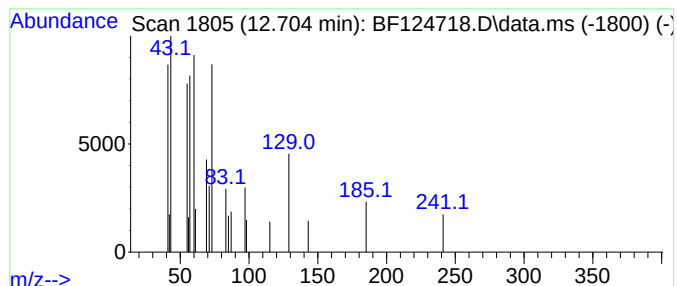
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Peak Number 4 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	6.04 ng	18197	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
2			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
3			n-Decanoic acid	172	C10H20O2	000334-48-5	59
4			Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	47
5			Undecanoic acid	186	C11H22O2	000112-37-8	47



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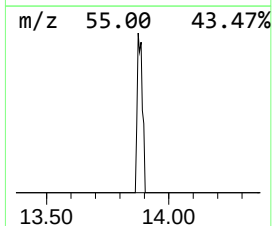
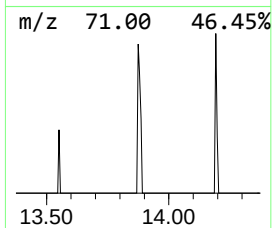
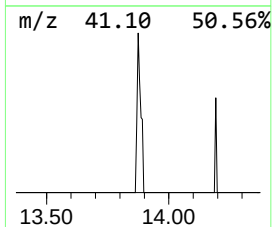
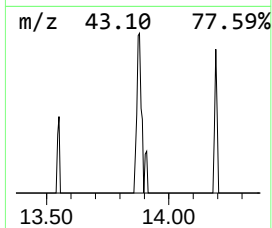
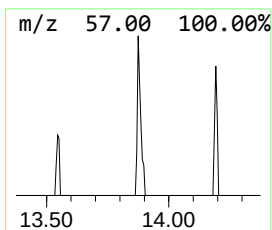
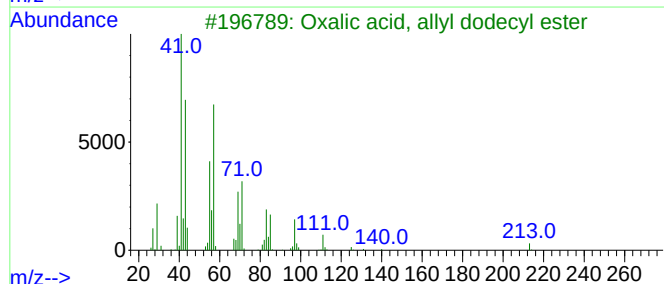
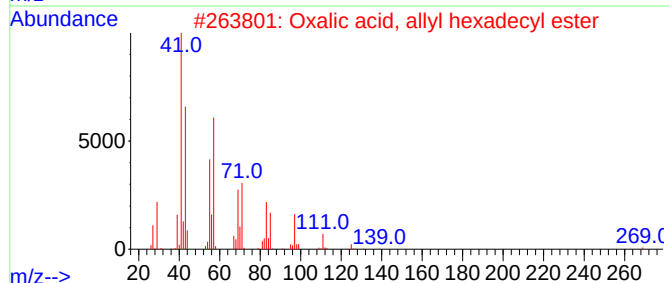
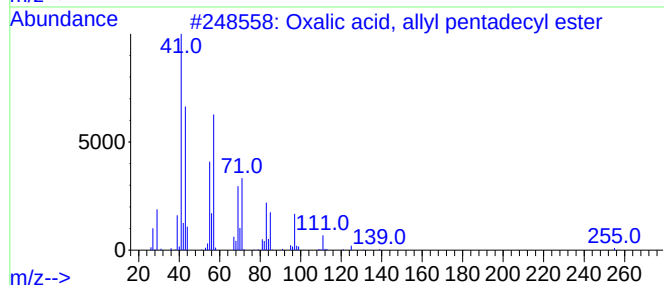
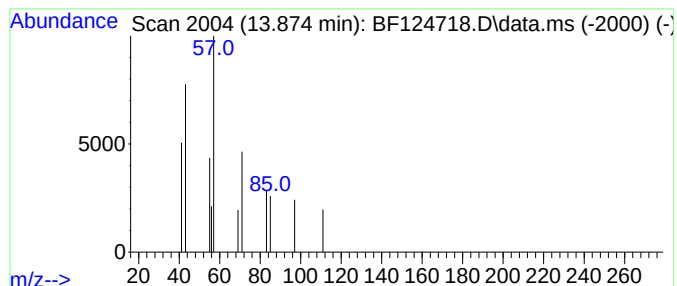
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Peak Number 5 Oxalic acid, allyl pentadec... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.21 ng	11708	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	72
2			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	72
3			Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	72
4			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	64
5			1-Decanol, 2-ethyl-	186	C12H26O	021078-65-9	64



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.181	6.2	ng	11140	1	6.869	36144	20.0
Ethanol, 2-(2-b...	8.051	13.3	ng	34076	2	8.151	51359	20.0
Undecanoic acid	11.916	9.5	ng	28672	4	11.392	60269	20.0
Tetradecanoic acid	12.704	6.0	ng	18197	4	11.392	60269	20.0
Oxalic acid, al...	13.874	5.2	ng	11708	5	14.027	44961	20.0