

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
 Data File : BF124743.D
 Acq On : 24 Jul 2021 12:47
 Operator : JU/CG
 Sample : M3152-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VAULT-A

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: BF124743.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	13012	15524	6.04%	1.028%
2	5.104	510	513	517	rBB	2635	3289	1.28%	0.218%
3	5.487	573	578	581	rBB	173173	180637	70.30%	11.956%
4	6.492	744	749	752	rBB	162212	184433	71.77%	12.207%
5	6.869	810	813	816	rBB	45172	32714	12.73%	2.165%
6	7.434	904	909	911	rBB	121463	122045	47.50%	8.078%
7	8.051	1011	1014	1017	rBB	18072	15216	5.92%	1.007%
8	8.151	1027	1031	1034	rBB	60204	48119	18.73%	3.185%
9	9.228	1209	1214	1217	rBV	275059	240164	93.46%	15.896%
10	9.904	1325	1329	1332	rBB	72627	60634	23.60%	4.013%
11	10.698	1459	1464	1467	rBB	194643	173980	67.71%	11.516%
12	11.392	1578	1582	1585	rBV	84539	65966	25.67%	4.366%
13	11.916	1667	1671	1675	rBB	25681	20600	8.02%	1.363%
14	12.598	1785	1787	1790	rBB	5595	4085	1.59%	0.270%
15	12.698	1802	1804	1806	rBB	12439	7929	3.09%	0.525%
16	12.827	1824	1826	1829	rBB	4777	3801	1.48%	0.252%
17	12.980	1848	1852	1855	rBB	279634	256963	100.00%	17.008%
18	13.874	2001	2004	2010	rBB	10388	12962	5.04%	0.858%
19	14.027	2026	2030	2033	rBV	45868	36498	14.20%	2.416%
20	15.498	2275	2280	2284	rBV2	22136	25267	9.83%	1.672%

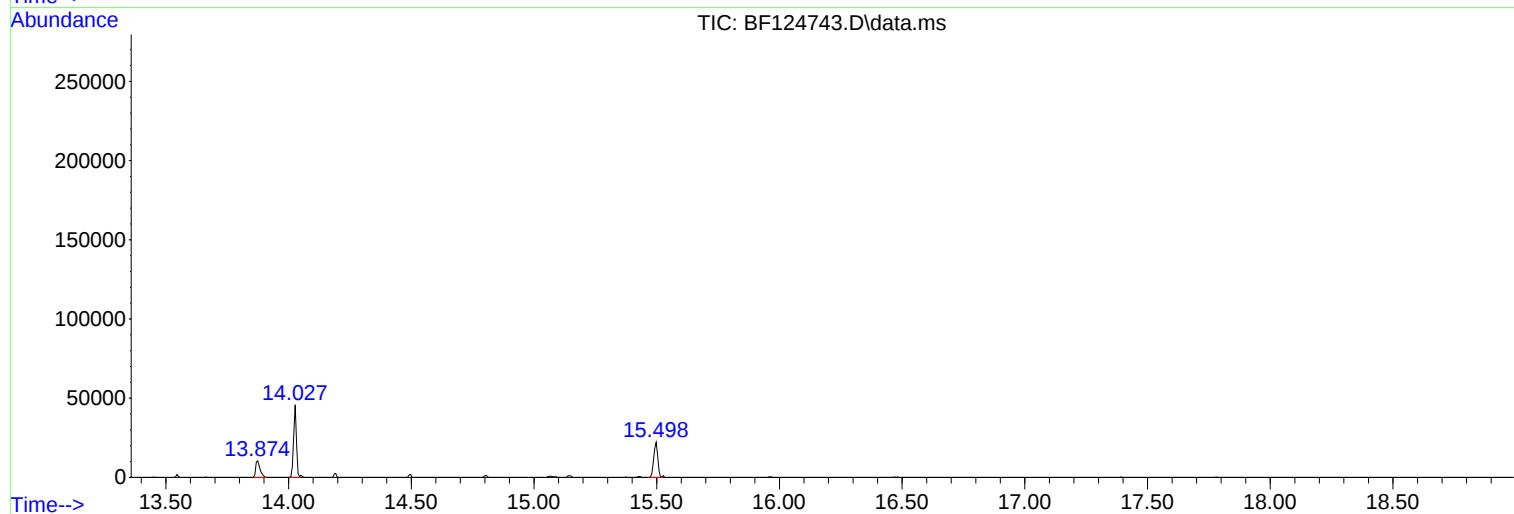
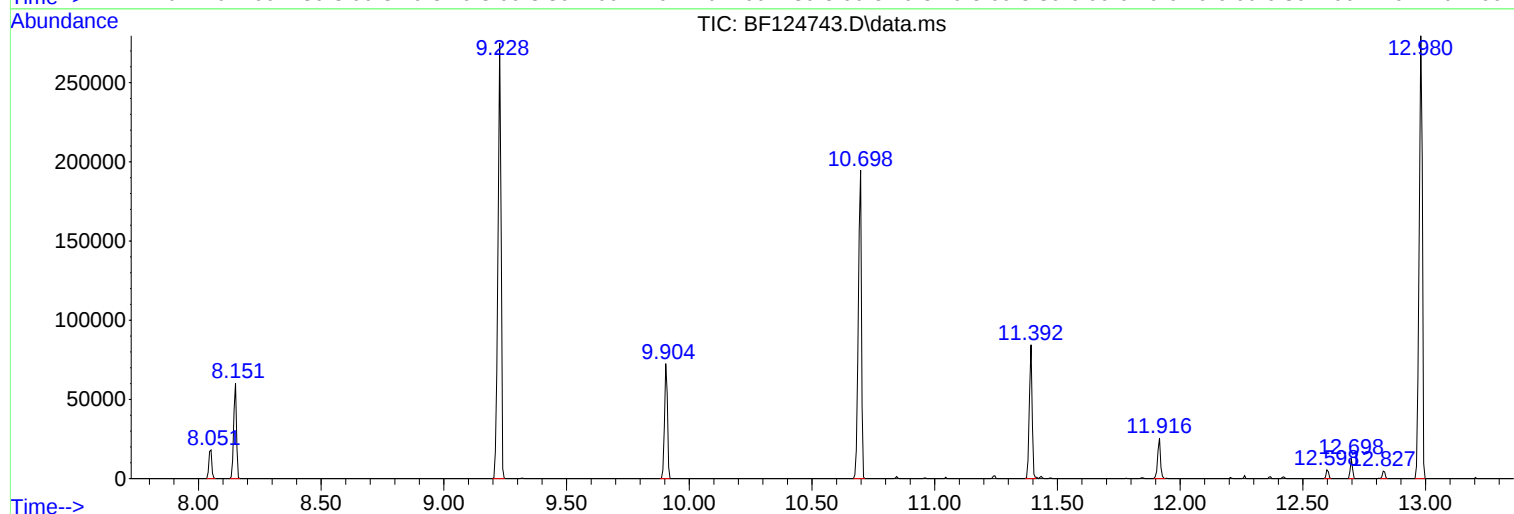
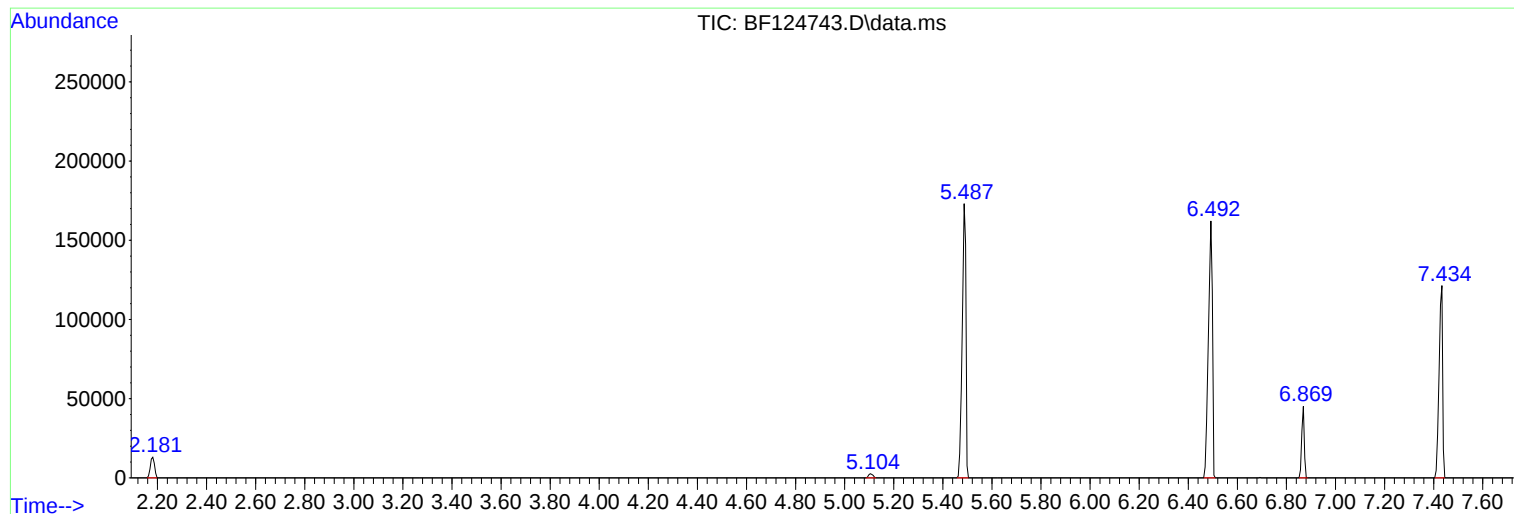
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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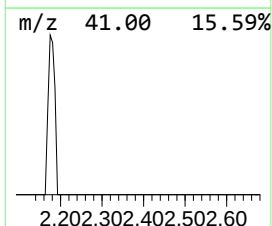
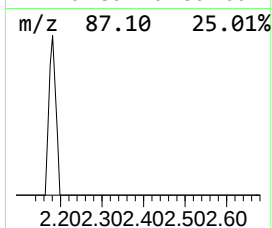
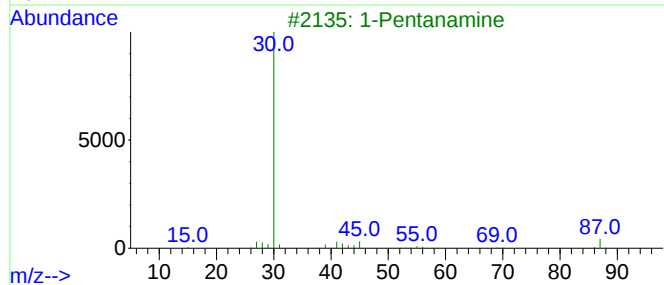
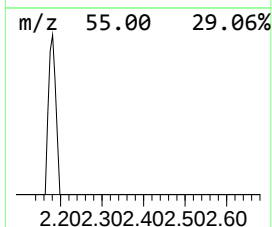
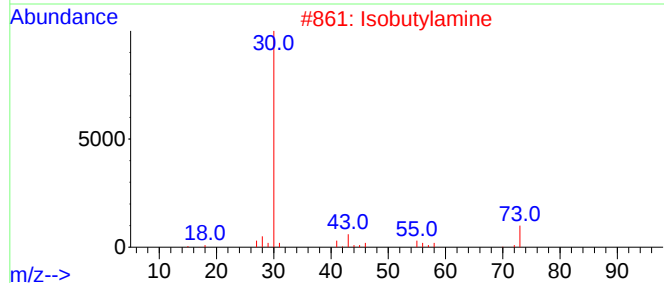
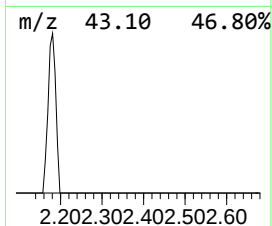
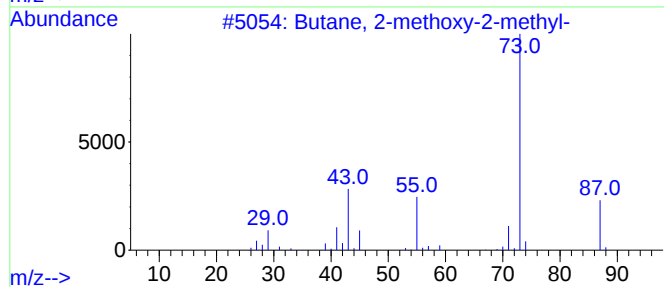
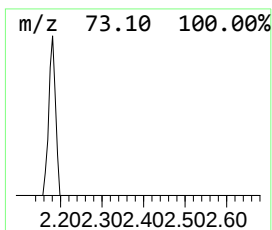
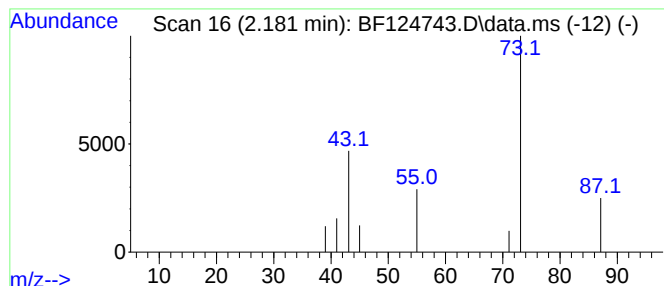
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.181	9.49 ng	15524	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	74
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4



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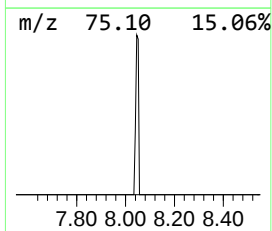
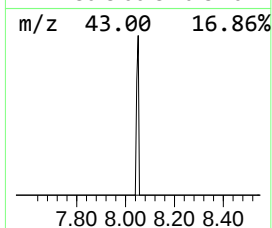
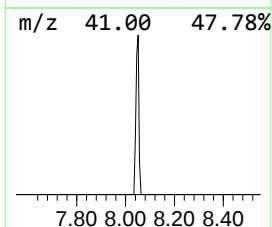
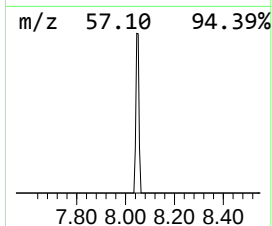
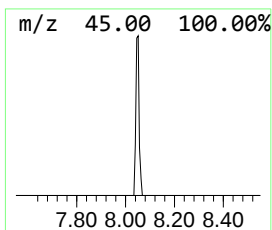
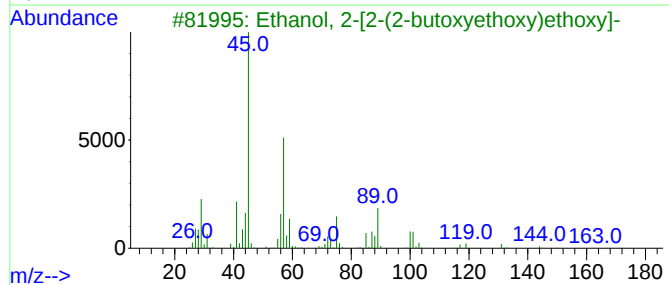
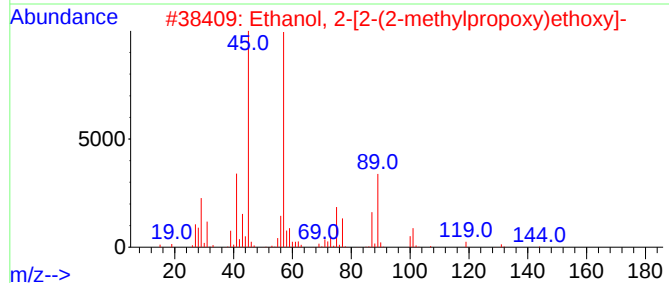
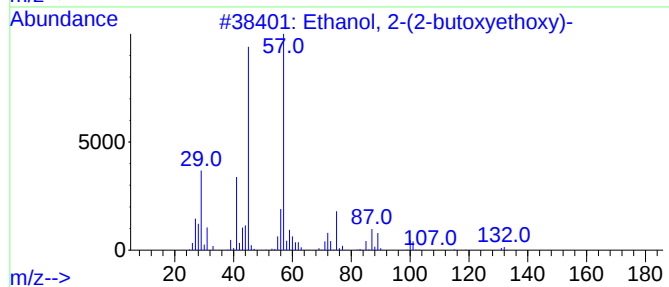
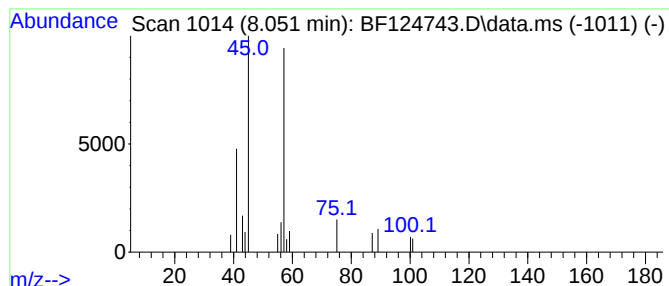
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	6.32 ng	15216	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	38
5			Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	17



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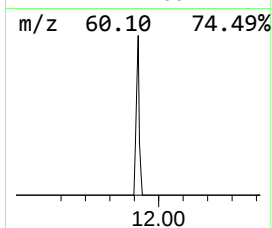
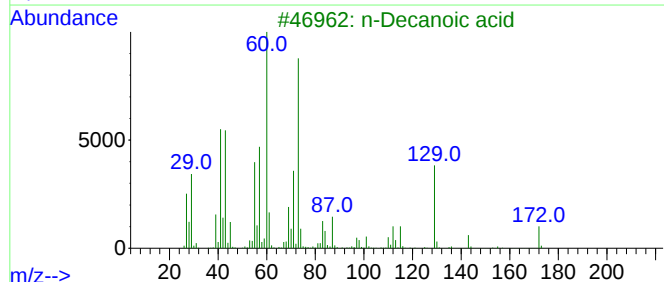
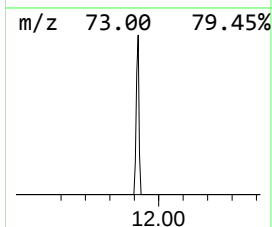
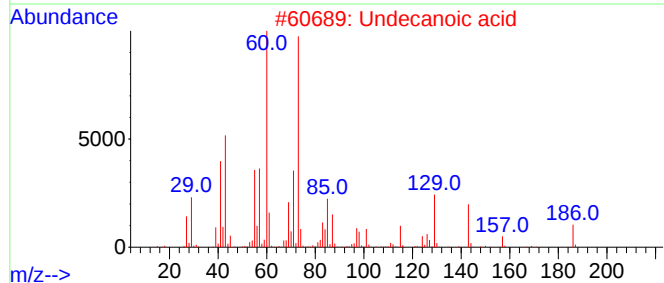
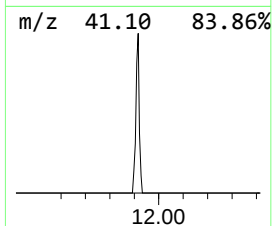
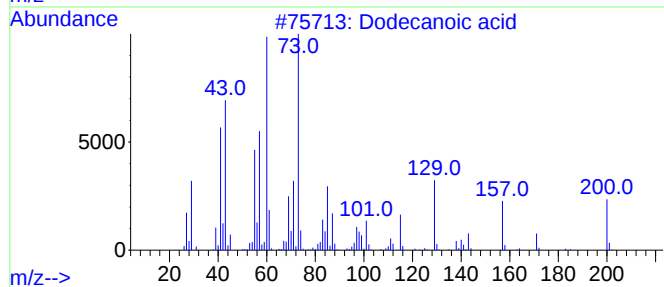
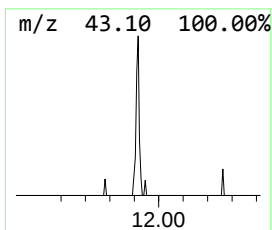
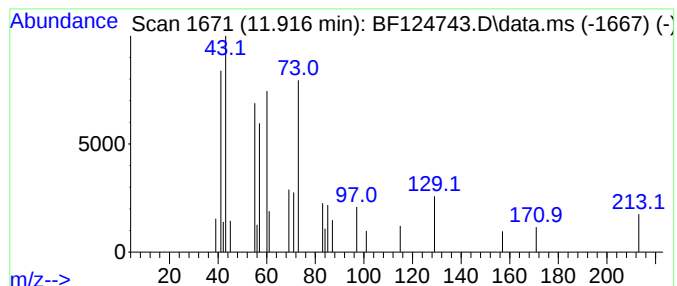
Instrument :
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.916	6.25 ng	20600	Phenanthrene-d10	11.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	72
2	Undecanoic acid	186	C11H22O2	000112-37-8	64
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	47
5	Octanoic acid	144	C8H16O2	000124-07-2	43



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VAULT-A

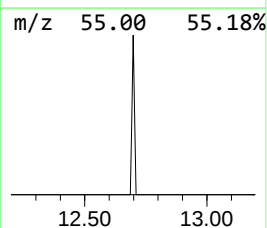
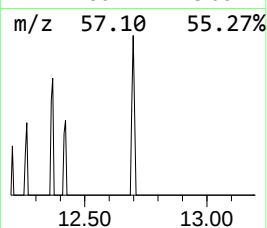
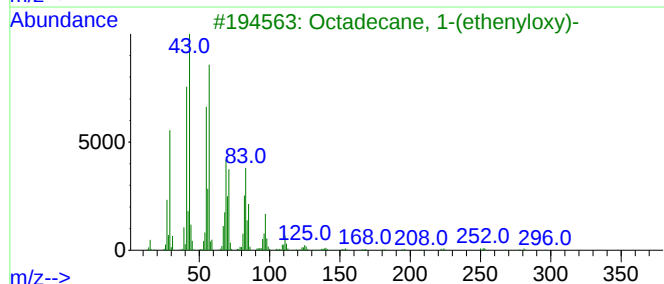
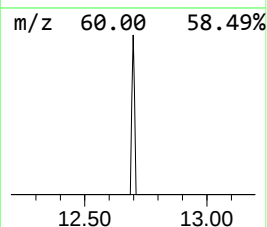
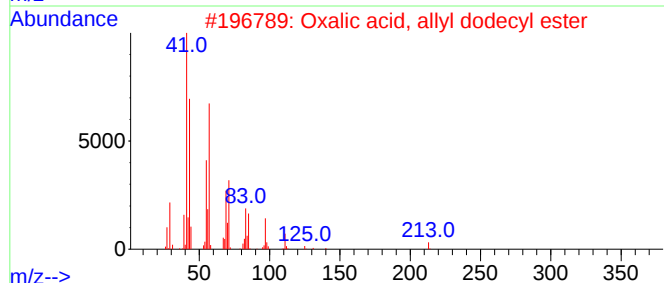
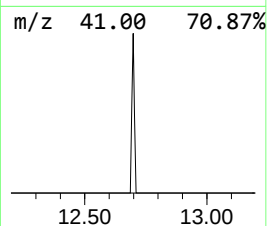
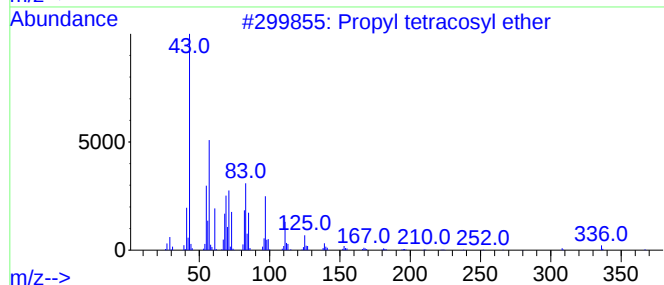
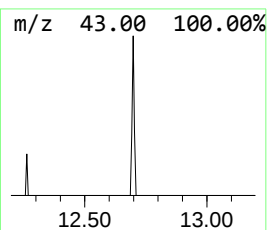
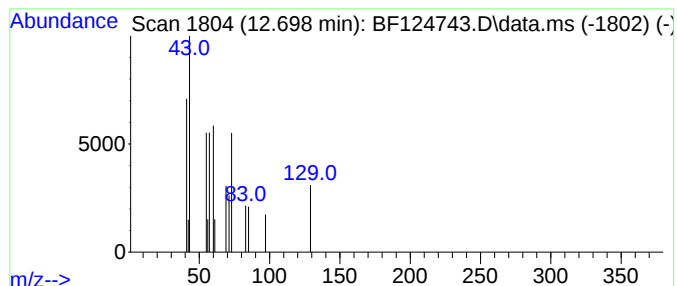
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Peak Number 5 unknown12.698 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	2.40 ng	7929	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propyl tetracosyl ether	396	C27H56O	1000406-28-3	43
2			Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	38
3			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	35
4			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	35
5			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	32



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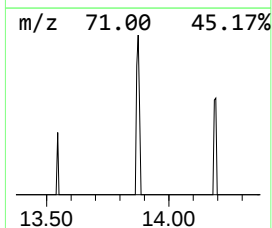
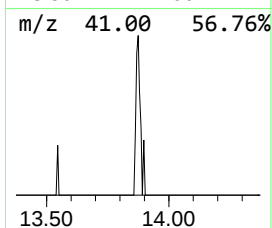
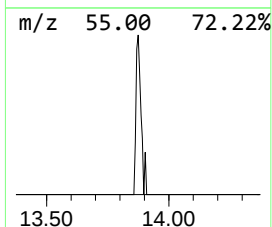
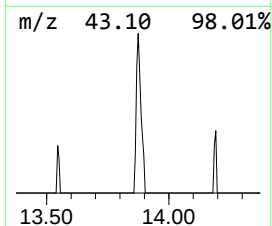
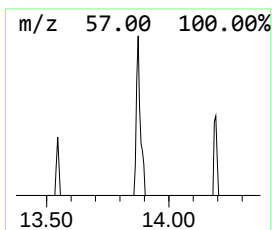
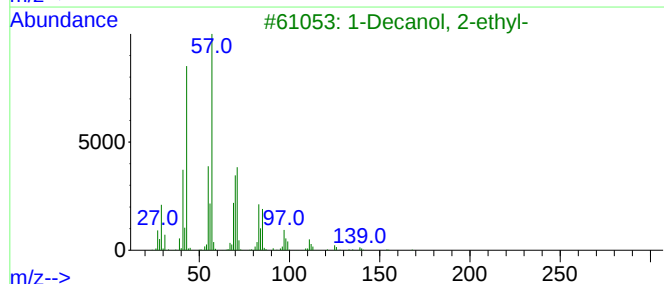
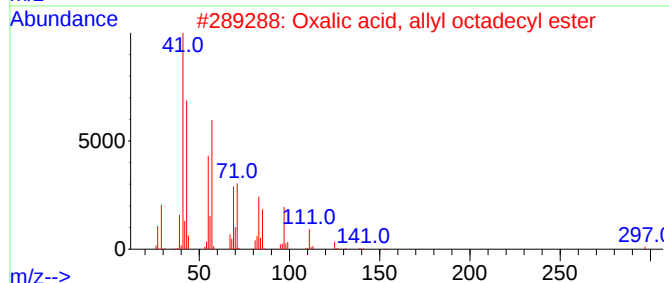
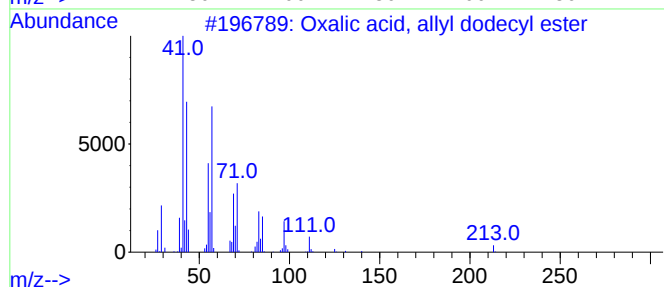
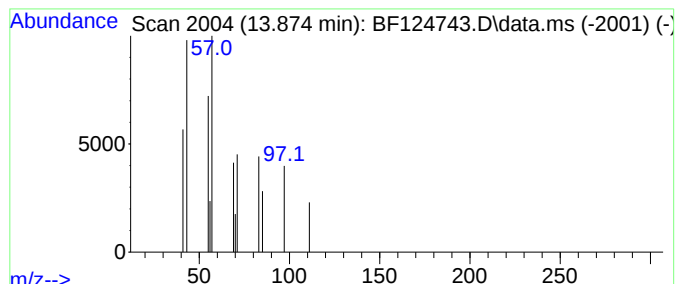
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Peak Number 7 Oxalic acid, allyl dodecyl ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	7.10 ng	12962	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	72
2			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	72
3			1-Decanol, 2-ethyl-	186	C12H26O	021078-65-9	64
4			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	59
5			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.181	9.5	ng	15524	1	6.869	32714	20.0
Ethanol, 2-(2-b...	8.051	6.3	ng	15216	2	8.151	48119	20.0
Dodecanoic acid	11.916	6.3	ng	20600	4	11.392	65966	20.0
unknown12.698	12.698	2.4	ng	7929	4	11.392	65966	20.0
Oxalic acid, al...	13.874	7.1	ng	12962	5	14.027	36498	20.0