

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
 Data File : BF124265.D
 Acq On : 11 Jun 2021 17:28
 Operator : JU/CG
 Sample : M2625-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 18-B12(138-142)

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124265.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	16	21	25	rBV	23097	29651	1.56%	0.287%
2	5.063	501	506	516	rBV	86635	119929	6.32%	1.163%
3	5.475	571	576	579	rBV	1443389	1276863	67.27%	12.378%
4	6.486	743	748	751	rBV	1317178	1261748	66.48%	12.231%
5	6.839	805	808	811	rBV	286784	209983	11.06%	2.036%
6	7.404	899	904	907	rBV	899566	865304	45.59%	8.388%
7	8.028	1007	1010	1019	rBV	34507	41787	2.20%	0.405%
8	8.122	1022	1026	1029	rBV	339056	271348	14.30%	2.630%
9	9.204	1205	1210	1213	rBV	1972607	1725300	90.90%	16.725%
10	9.880	1321	1325	1328	rBV	429528	336643	17.74%	3.263%
11	10.674	1455	1460	1463	rBV	1388246	1263454	66.57%	12.248%
12	11.368	1574	1578	1581	rBV	419112	362134	19.08%	3.511%
13	11.892	1664	1667	1670	rBV	43959	37564	1.98%	0.364%
14	12.957	1843	1848	1851	rBV	2095456	1898061	100.00%	18.400%
15	13.868	1995	2003	2011	rBV6	30776	71563	3.77%	0.694%
16	14.009	2023	2027	2031	rVB	294465	260561	13.73%	2.526%
17	14.862	2167	2172	2176	rVB2	20858	24266	1.28%	0.235%
18	15.486	2273	2278	2285	rVB	192901	259461	13.67%	2.515%

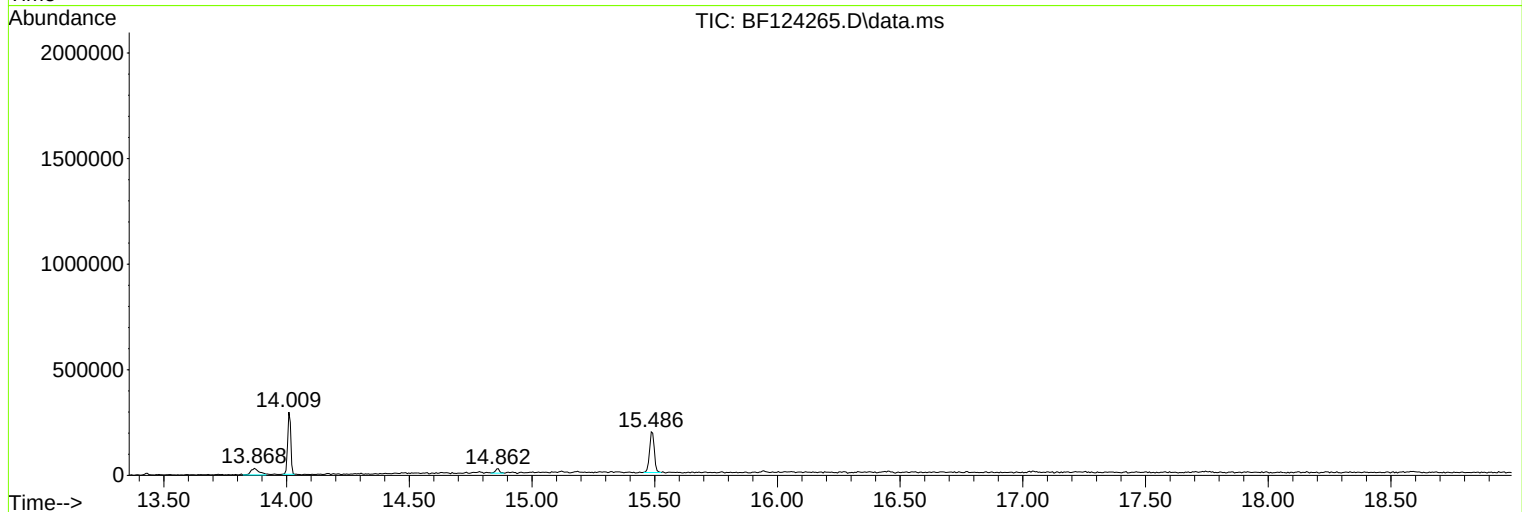
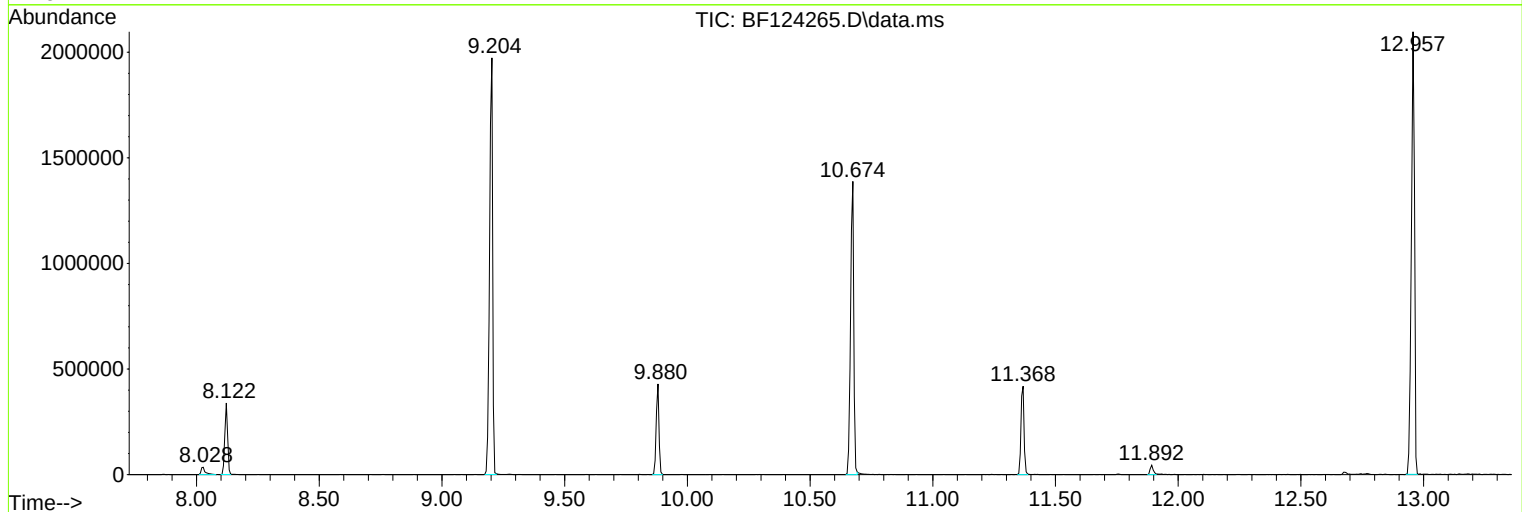
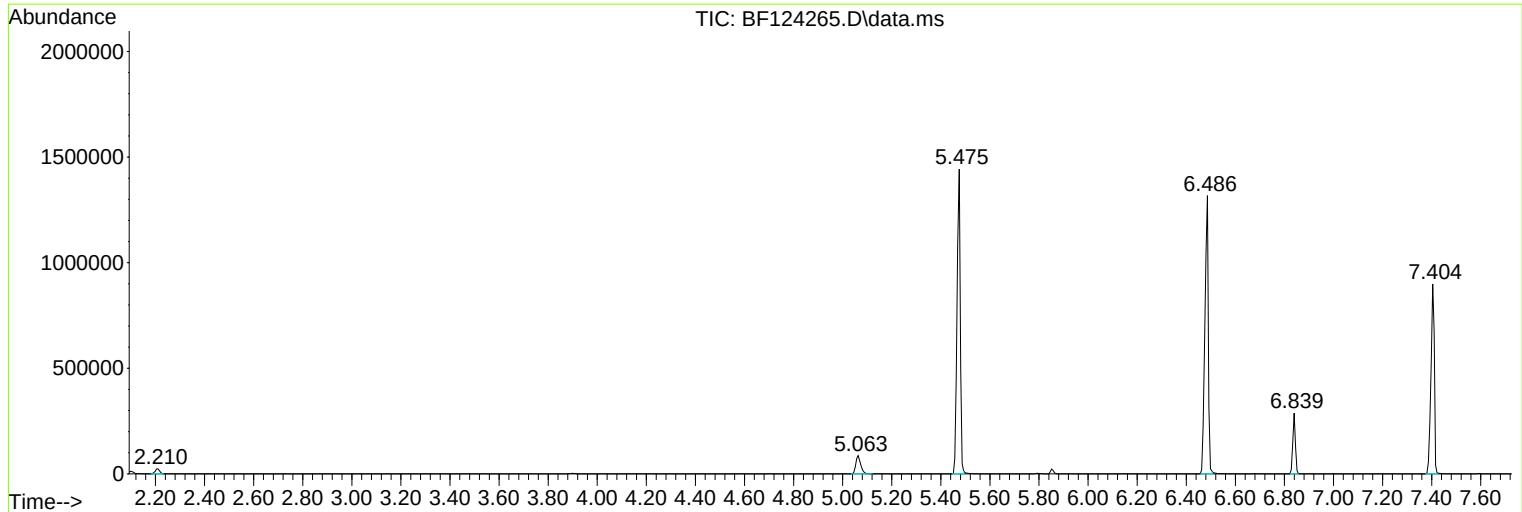
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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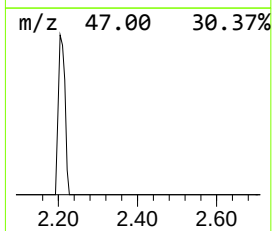
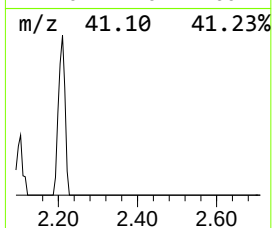
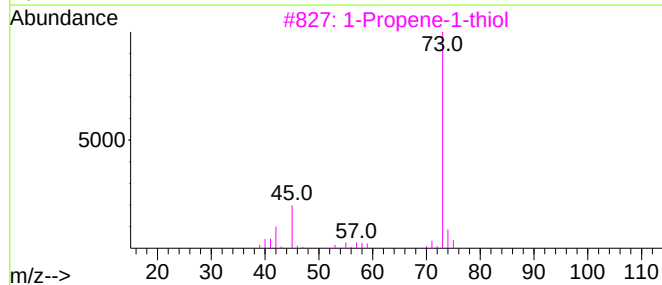
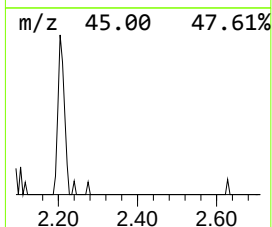
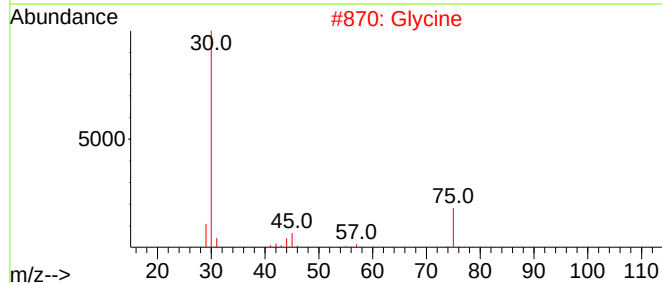
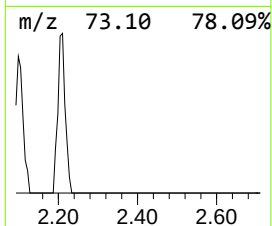
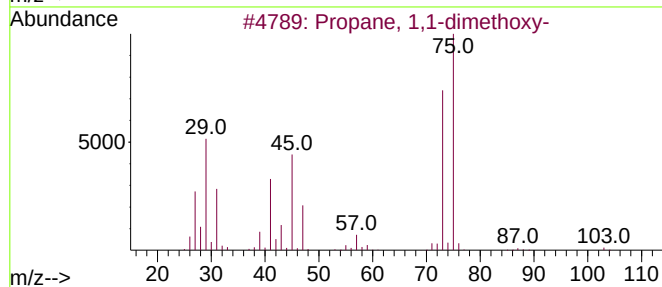
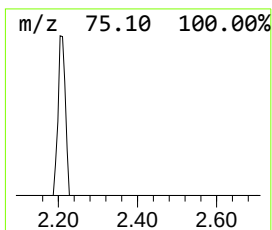
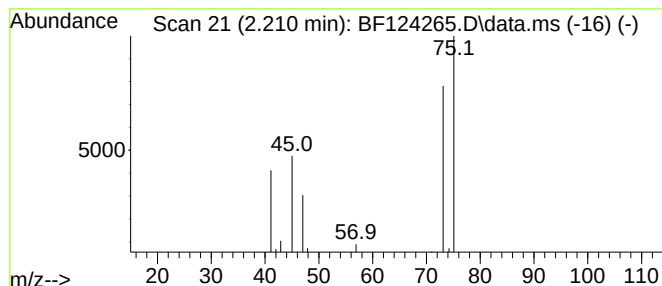
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	2.82 ng	29651	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Glycine	75	C2H5NO2	000056-40-6	5
3			1-Propene-1-thiol	74	C3H6S	000925-89-3	5
4			Methane, nitroso-	45	CH3NO	000865-40-7	4
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	4



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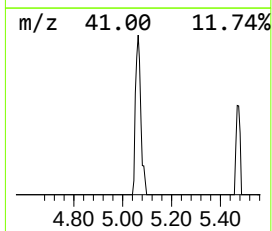
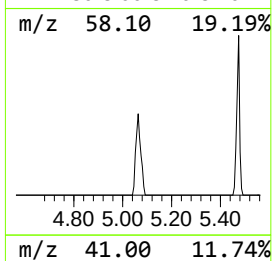
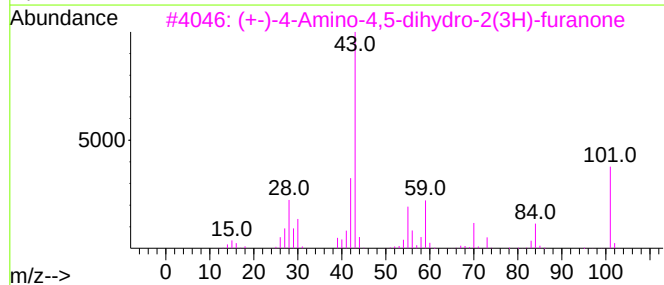
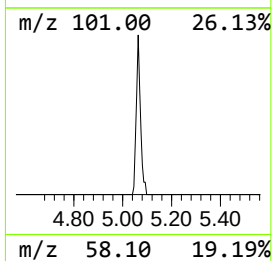
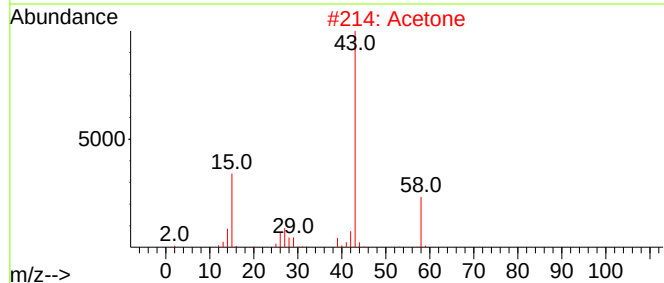
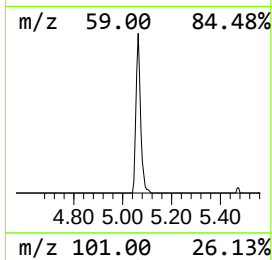
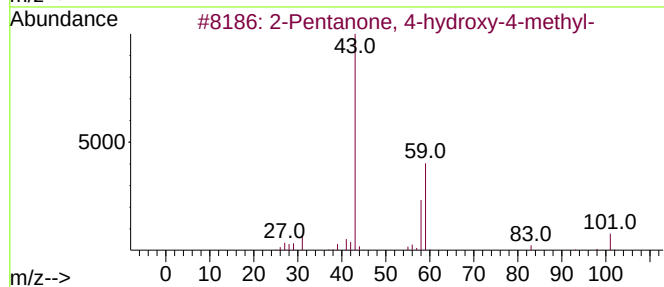
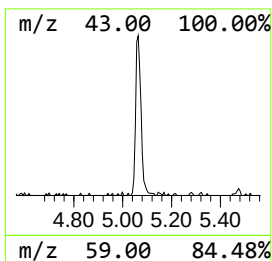
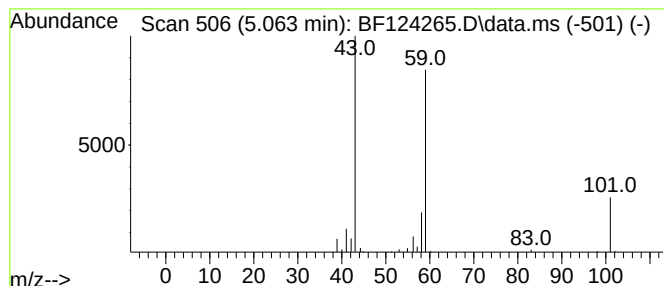
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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.
5.063	11.42 ng	119929	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetone	58	C3H6O	000067-64-1	9
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Guanidine	59	CH5N3	000113-00-8	9



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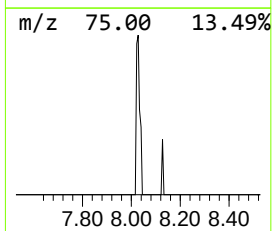
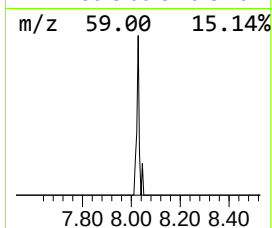
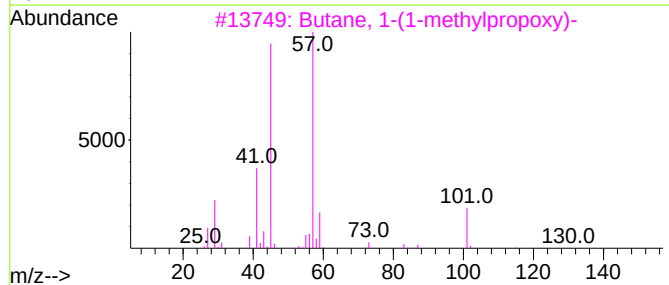
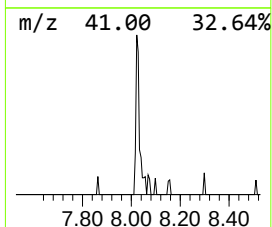
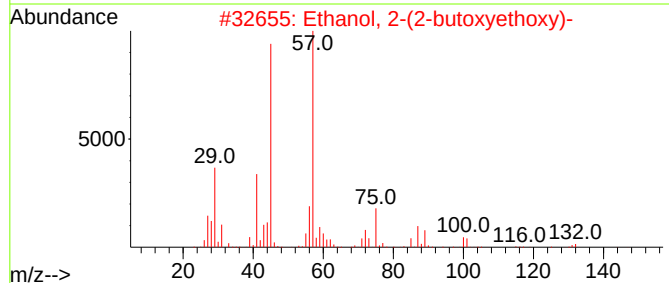
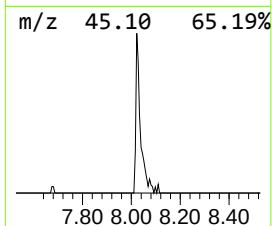
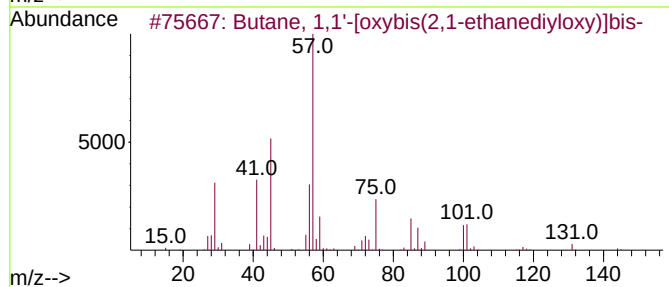
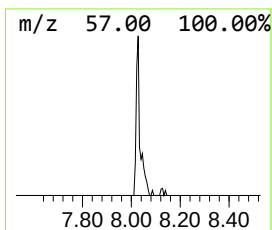
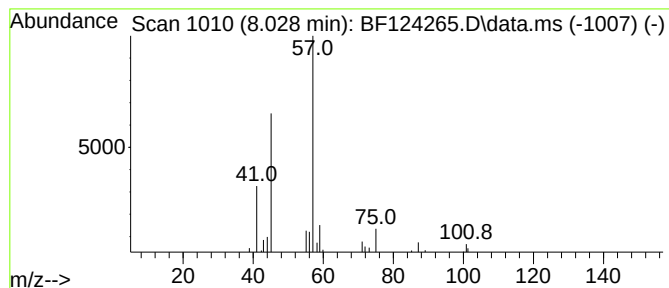
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Butane, 1,1'-[oxybis(2,1-et... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.028	3.08 ng	41787	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	64		
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	59		
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	45		
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	42		
5	Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	36		



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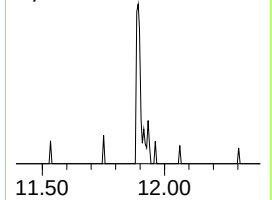
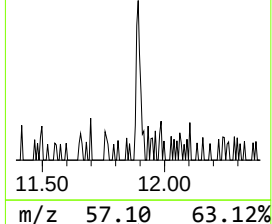
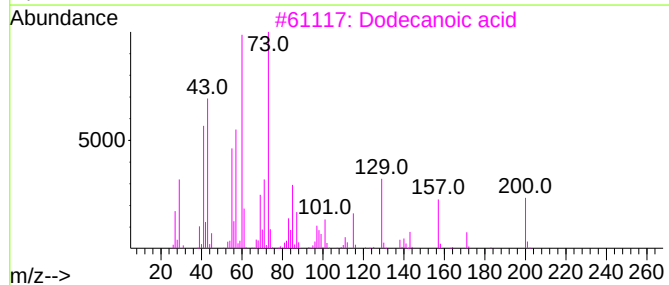
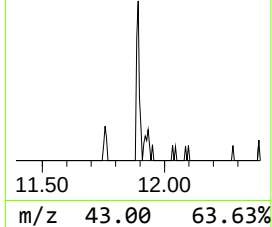
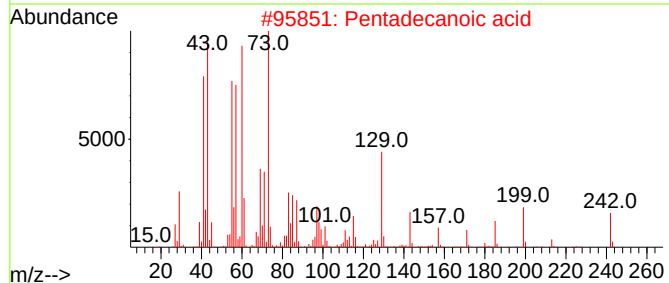
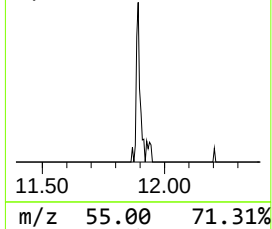
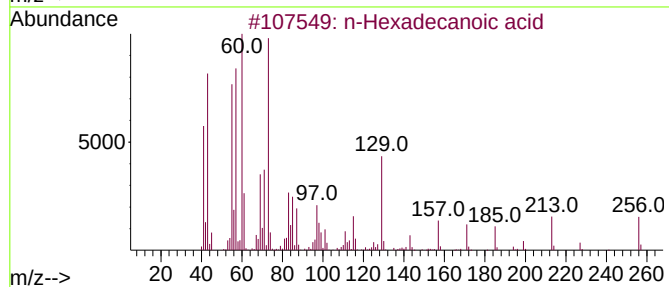
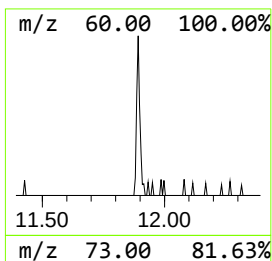
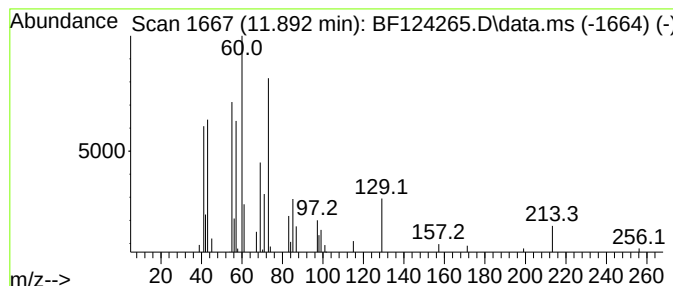
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	2.07 ng	37564	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Dodecanoic acid	200	C12H24O2	000143-07-7	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	59
5			Undecanoic acid	186	C11H22O2	000112-37-8	59



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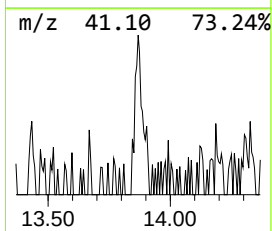
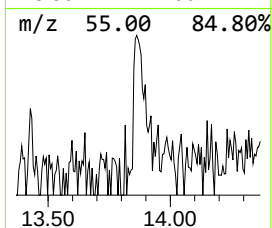
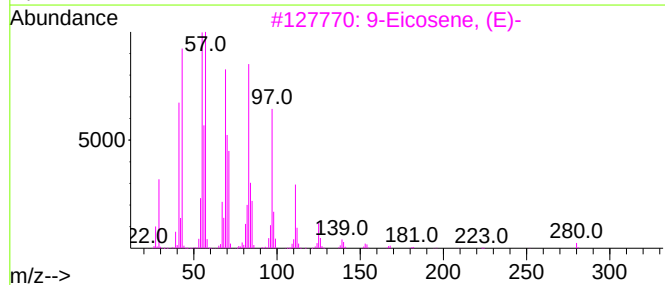
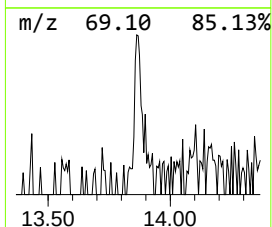
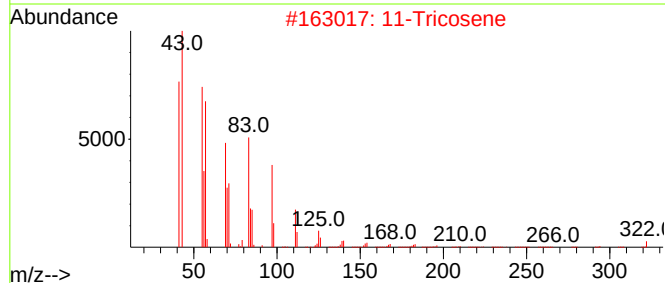
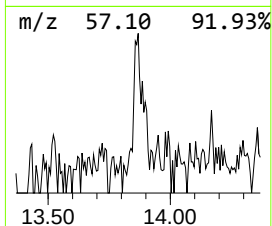
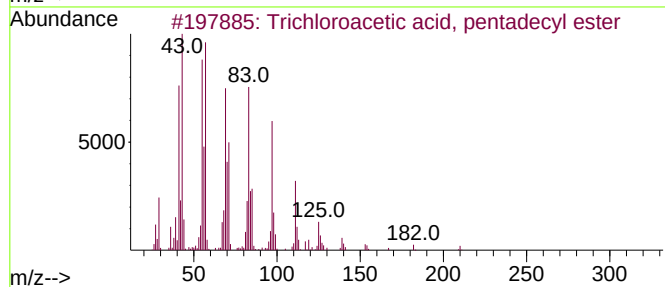
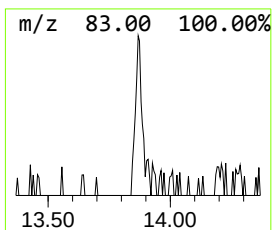
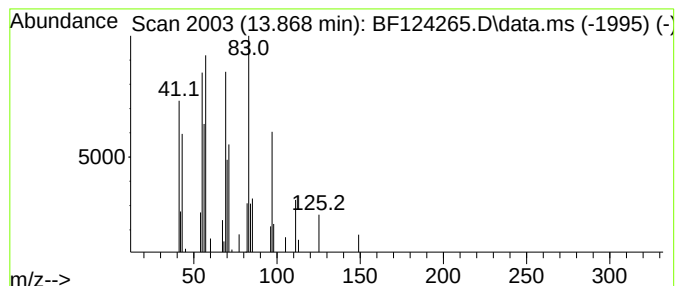
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	5.49 ng	71563	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2			11-Tricosene	322	C23H46	052078-56-5	86
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	83
4			1-Hexadecanol	242	C16H34O	036653-82-4	80
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	80



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-di...	2.210	2.8	ng	29651	1	6.839	209983	20.0
2-Pentanone, 4-...	5.063	11.4	ng	119929	1	6.839	209983	20.0
Butane, 1,1'-[o...	8.028	3.1	ng	41787	2	8.122	271348	20.0
n-Hexadecanoic ...	11.892	2.1	ng	37564	4	11.368	362134	20.0
Trichloroacetic...	13.868	5.5	ng	71563	5	14.009	260561	20.0