

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062321\
 Data File : BP006034.D
 Acq On : 23 Jun 2021 14:45
 Operator : CG/JU
 Sample : M2773-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-4

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_P\Methods\8270E-BP060821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006034.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.417	222	226	238	rVB	27342	41322	1.27%	0.288%
2	5.022	324	329	343	rBV	71825	110086	3.38%	0.768%
3	5.493	402	409	427	rBV	748792	1170078	35.90%	8.163%
4	7.093	674	681	703	rBV	666885	1169788	35.89%	8.161%
5	7.916	814	821	830	rBV	230612	375039	11.51%	2.617%
6	9.081	1012	1019	1035	rBV	392736	730897	22.42%	5.099%
7	10.528	1256	1265	1279	rBV	22370	72460	2.22%	0.506%
8	10.722	1291	1298	1308	rBV	276625	489113	15.00%	3.412%
9	13.175	1708	1715	1731	rBV	1237334	1792202	54.98%	12.504%
10	14.545	1940	1948	1963	rBV	402616	646090	19.82%	4.508%
11	16.039	2191	2202	2218	rBV	633832	1089116	33.41%	7.599%
12	17.292	2409	2415	2430	rBV	478255	787484	24.16%	5.494%
13	17.957	2524	2528	2536	rBV	29065	37116	1.14%	0.259%
14	18.175	2561	2565	2575	rBV3	30165	57940	1.78%	0.404%
15	19.086	2716	2720	2729	rVB2	83446	104728	3.21%	0.731%
16	19.304	2752	2757	2763	rBV	22986	37513	1.15%	0.262%
17	19.839	2843	2848	2862	rBV	2642411	3259704	100.00%	22.743%
18	21.069	3054	3057	3067	rBV6	47791	114069	3.50%	0.796%
19	21.369	3102	3108	3113	rBV	735802	1085143	33.29%	7.571%
20	23.768	3510	3516	3529	rVB2	541504	1163162	35.68%	8.115%

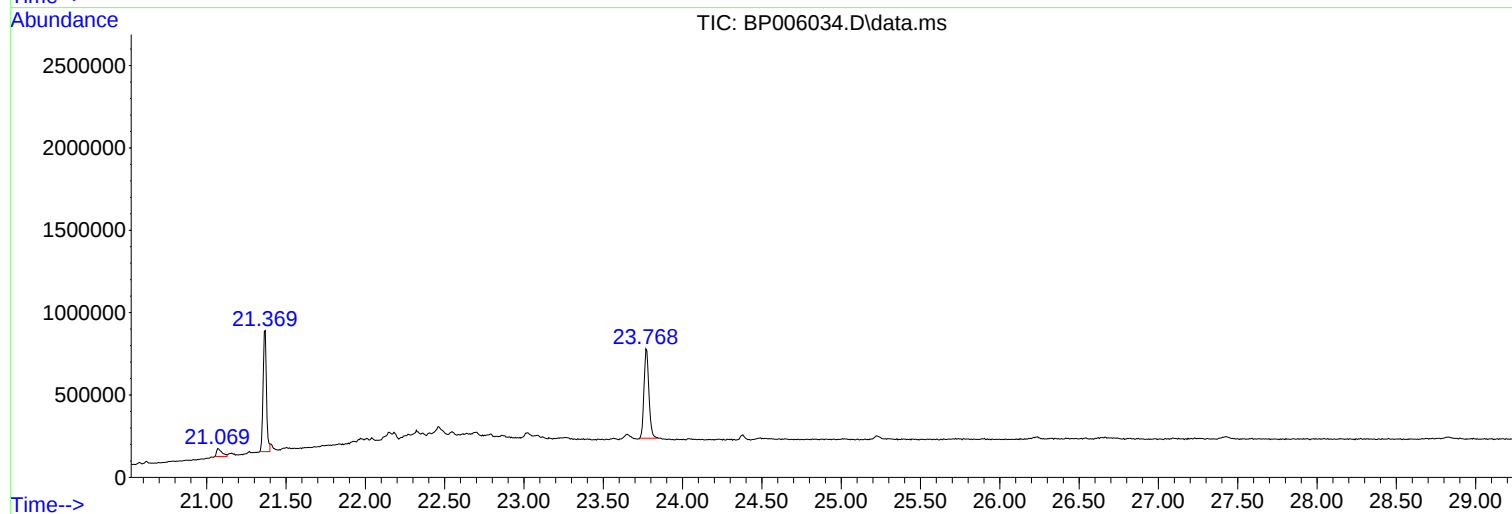
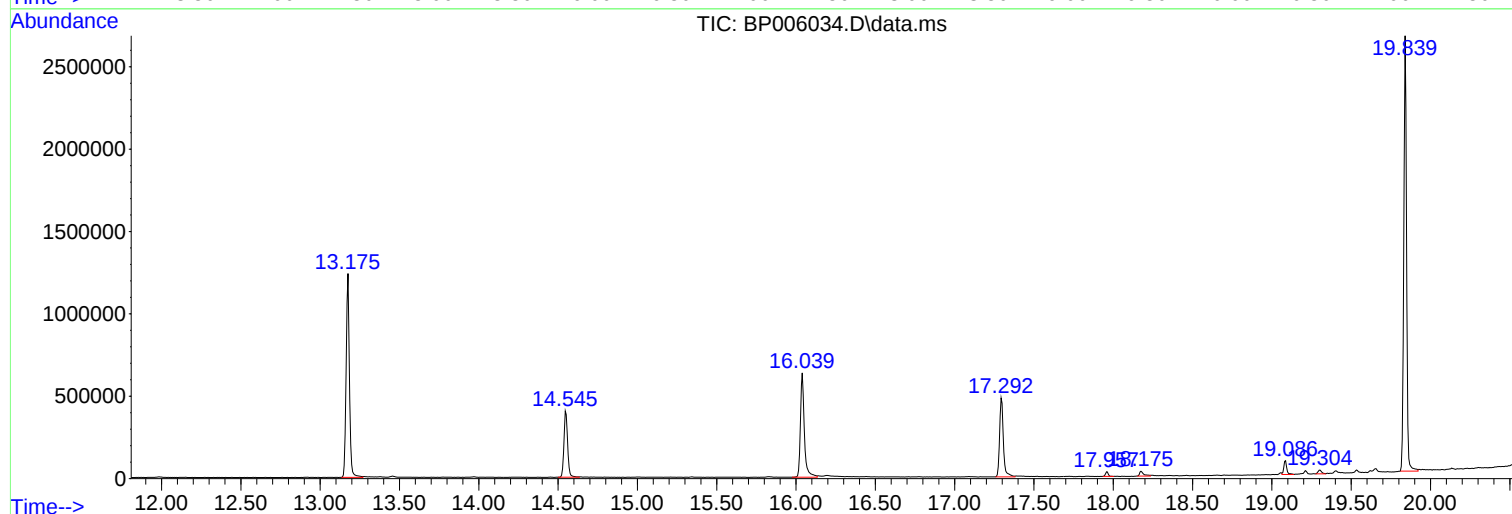
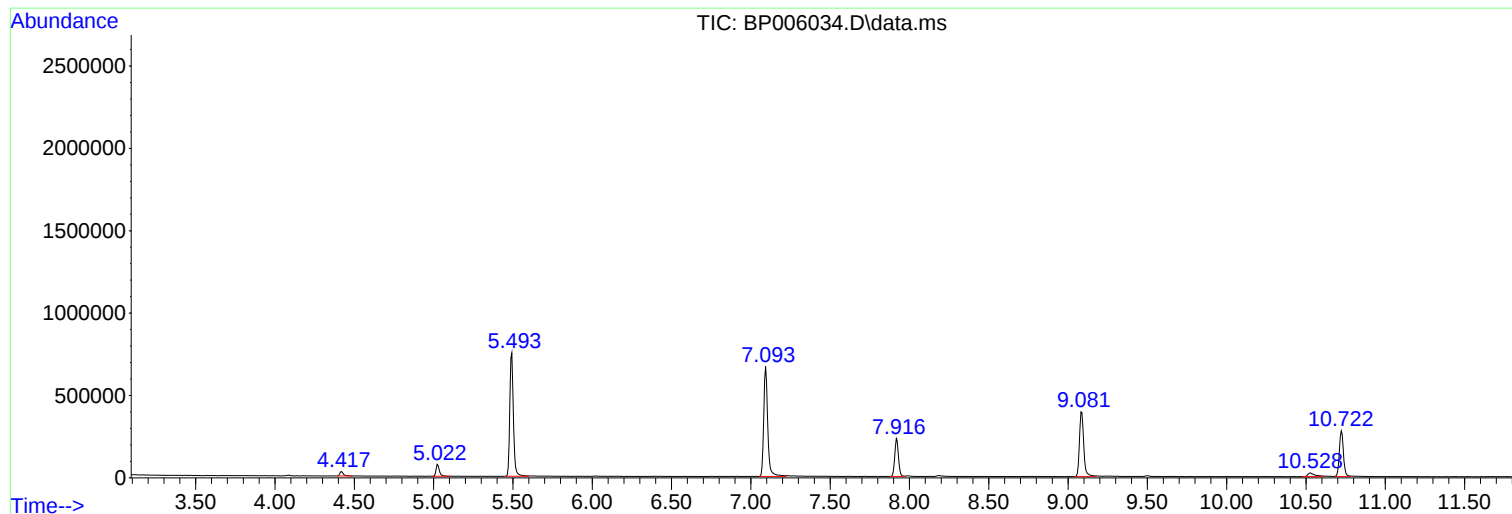
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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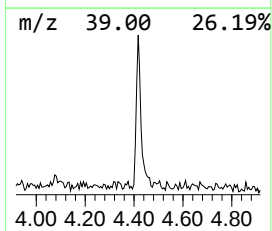
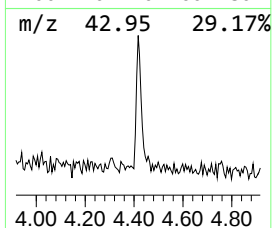
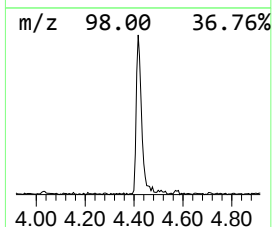
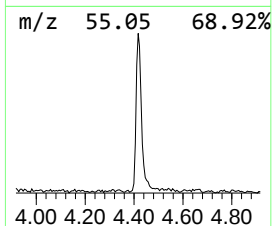
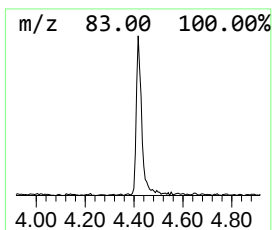
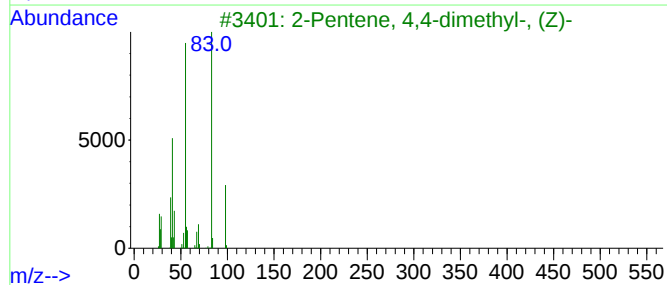
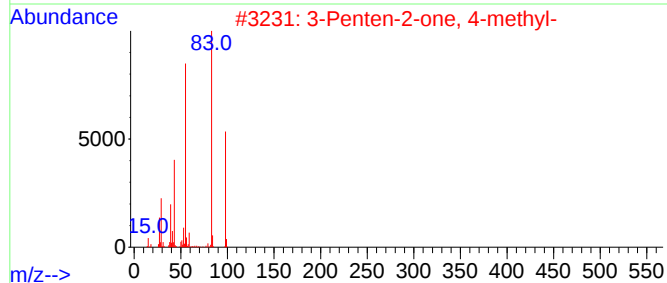
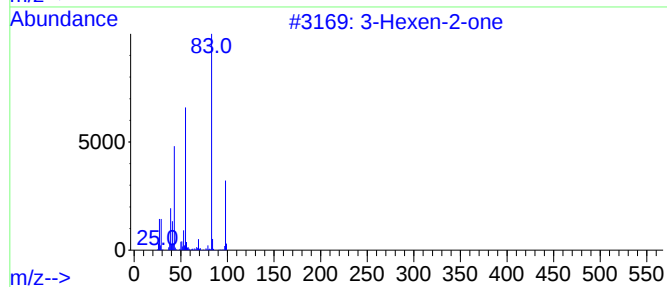
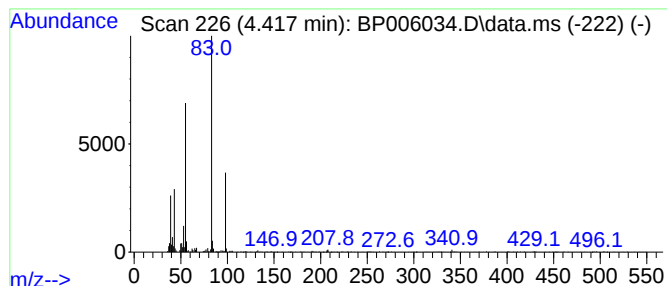
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.417	2.20 ng	41322	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	74
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	72
3			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	64
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	50



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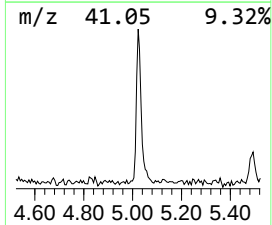
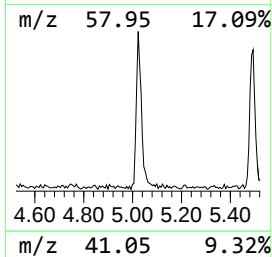
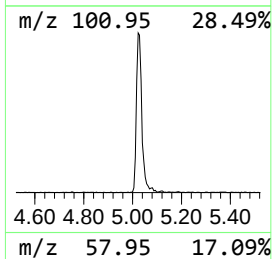
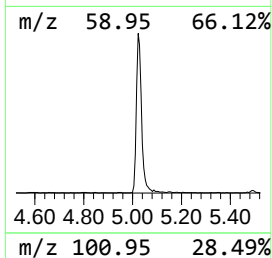
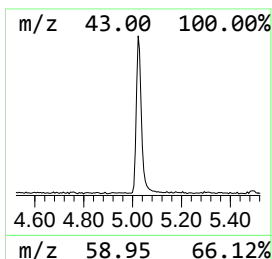
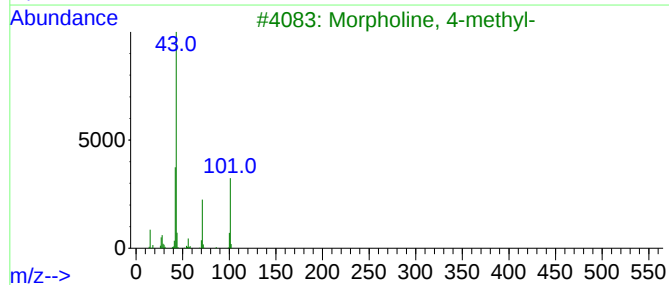
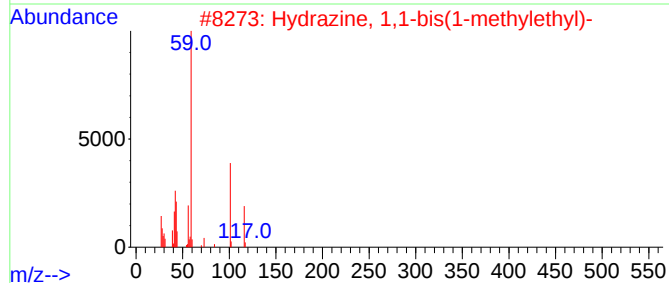
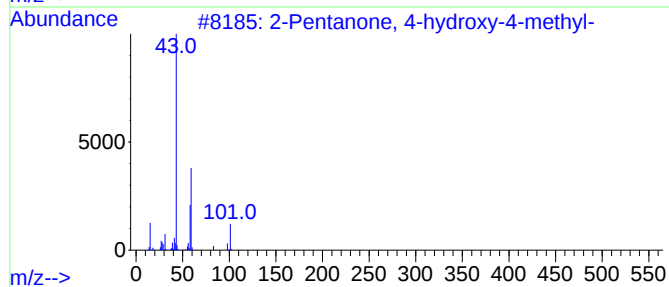
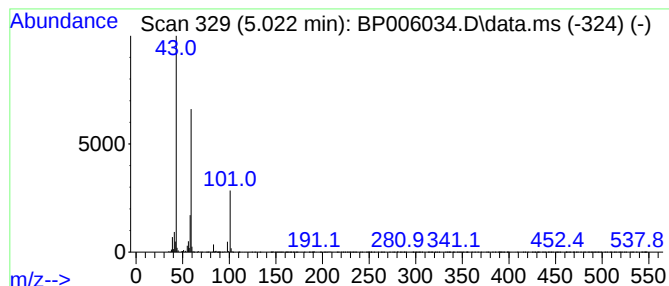
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	5.87 ng	110086	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9



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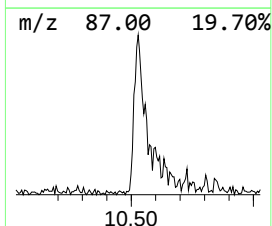
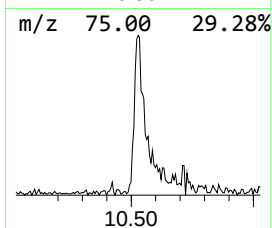
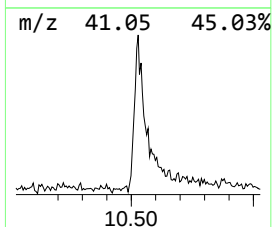
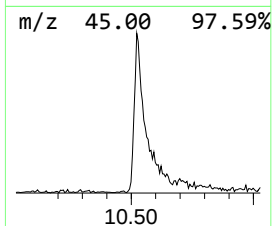
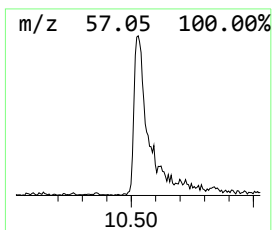
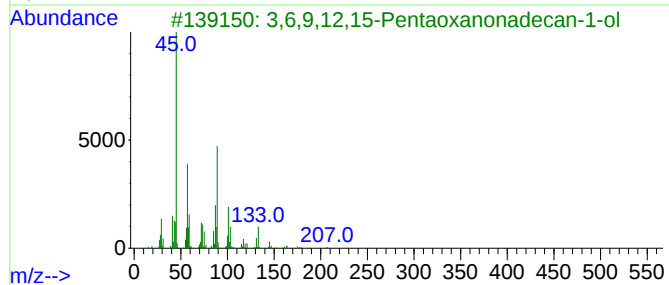
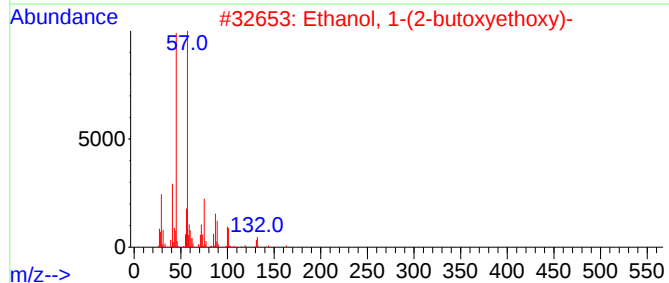
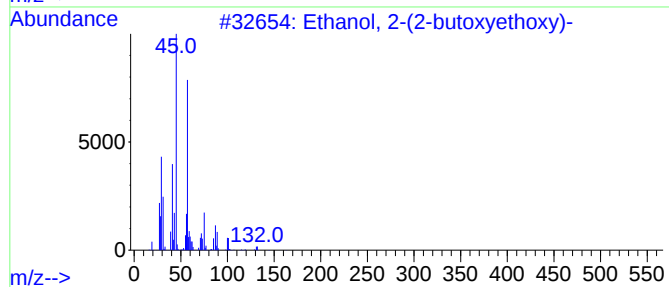
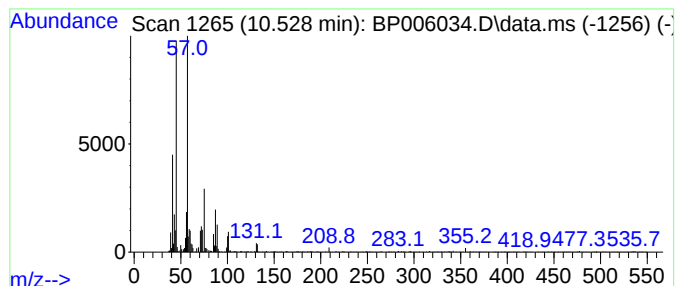
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.528	2.96 ng	72460	Naphthalene-d8	10.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	64
3			3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	59
4			2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	59
5			Diisopropyl ether	102	C6H14O	000108-20-3	59



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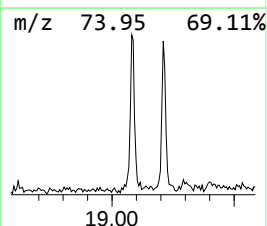
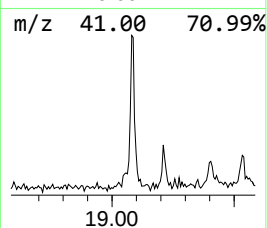
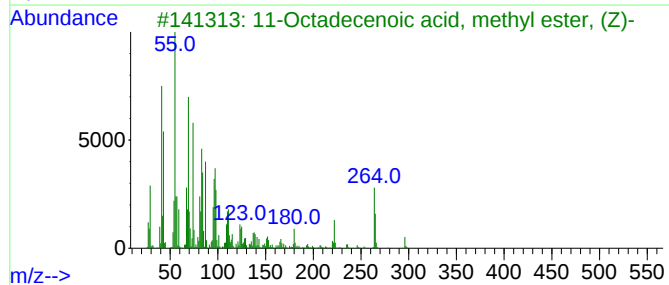
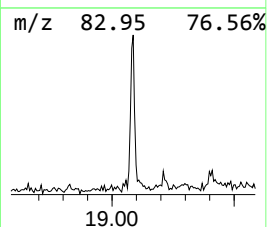
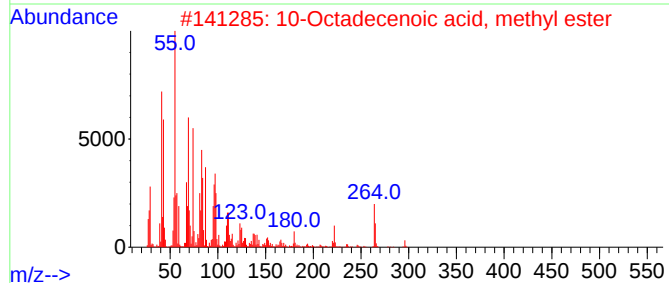
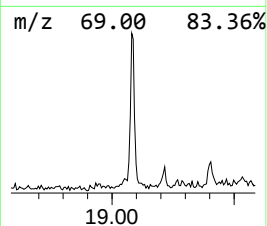
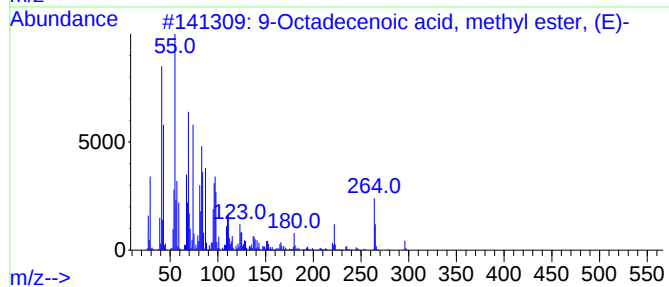
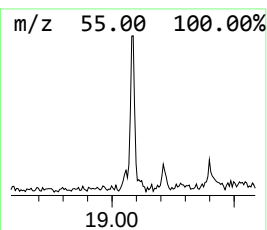
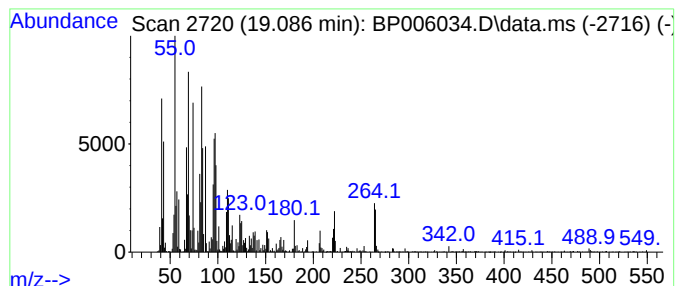
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 9-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.086	2.66 ng	104728	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
2			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98
5			9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	97



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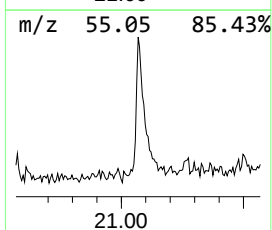
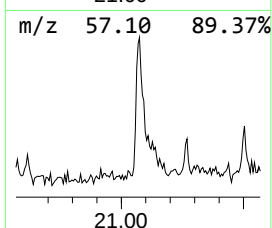
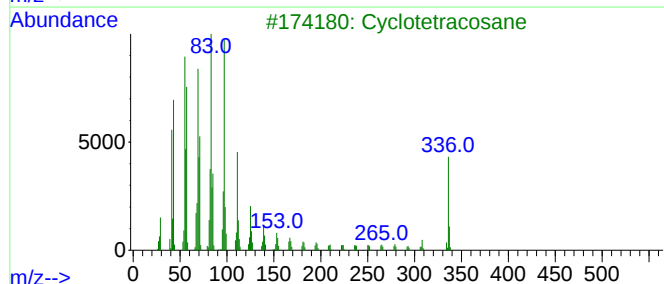
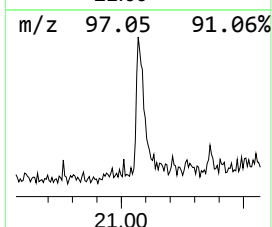
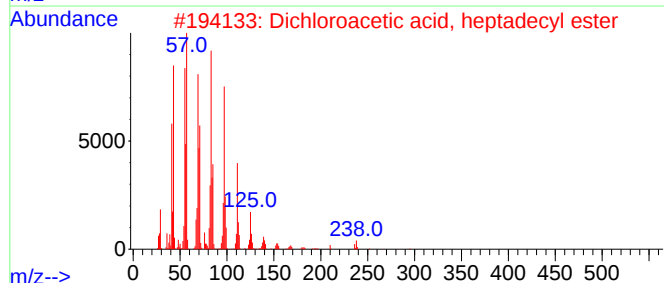
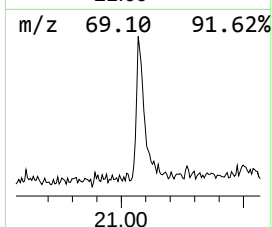
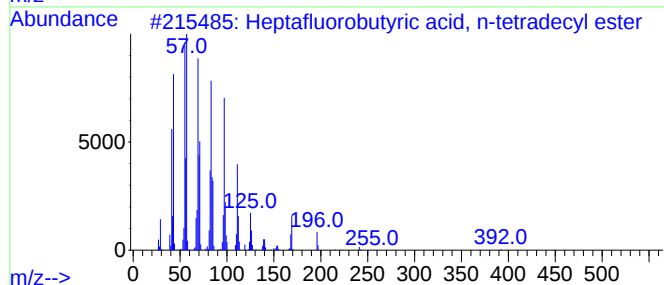
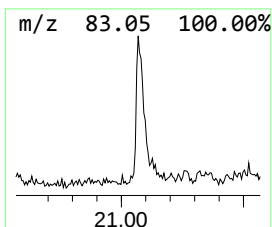
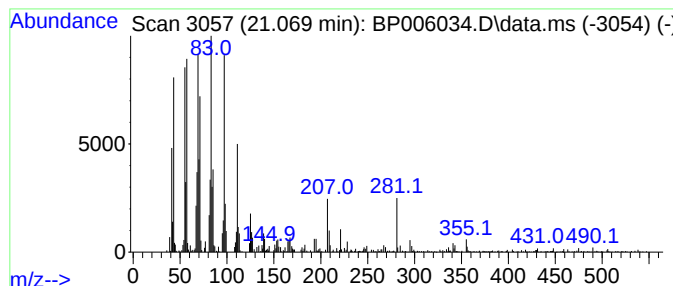
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.069	2.10 ng	114069	Chrysene-d12	21.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
3			Cyclotetracosane	336	C24H48	000297-03-0	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.417	2.2	ng	41322	1	7.916	375039	20.0
2-Pentanone, 4-...	5.022	5.9	ng	110086	1	7.916	375039	20.0
Ethanol, 2-(2-b...	10.528	3.0	ng	72460	2	10.722	489113	20.0
9-Octadecenoic ...	19.086	2.7	ng	104728	4	17.292	787484	20.0
Heptafluorobuty...	21.069	2.1	ng	114069	5	21.369	1085140	20.0