

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111621\
 Data File : BG051051.D
 Acq On : 15 Nov 2021 21:27
 Operator : CG/JU
 Sample : M4681-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-1

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_G\Methods\8270-BG111321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051051.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.290	300	307	316	rBV	269134	418555	11.93%	2.463%
2	5.760	379	387	398	rBV	996508	1623884	46.29%	9.555%
3	7.376	653	662	675	rBV	1012293	1813846	51.71%	10.672%
4	8.222	799	806	813	rBV	141562	245940	7.01%	1.447%
5	9.403	998	1007	1014	rBV	619273	1145405	32.65%	6.739%
6	10.801	1236	1245	1262	rBV	166785	330478	9.42%	1.944%
7	11.048	1280	1287	1295	rBV	202339	378331	10.79%	2.226%
8	13.475	1690	1700	1709	rBV	1588262	2502575	71.34%	14.725%
9	14.850	1928	1934	1946	rVB	357401	574576	16.38%	3.381%
10	16.336	2181	2187	2200	rVB	1260241	2016399	57.48%	11.864%
11	17.599	2395	2402	2409	rBV	456079	704652	20.09%	4.146%
12	18.228	2504	2509	2515	rVB	46439	62284	1.78%	0.366%
13	18.445	2541	2546	2552	rBV	51676	76745	2.19%	0.452%
14	19.385	2702	2706	2710	rVB2	67046	77024	2.20%	0.453%
15	19.709	2757	2761	2770	rBV3	28838	48377	1.38%	0.285%
16	20.190	2836	2843	2848	rBV	2603965	3507884	100.00%	20.640%
17	21.489	3059	3064	3077	rVB2	82858	169674	4.84%	0.998%
18	21.894	3127	3133	3144	rVB2	364161	645873	18.41%	3.800%
19	25.302	3703	3713	3724	rVB3	199528	653411	18.63%	3.845%

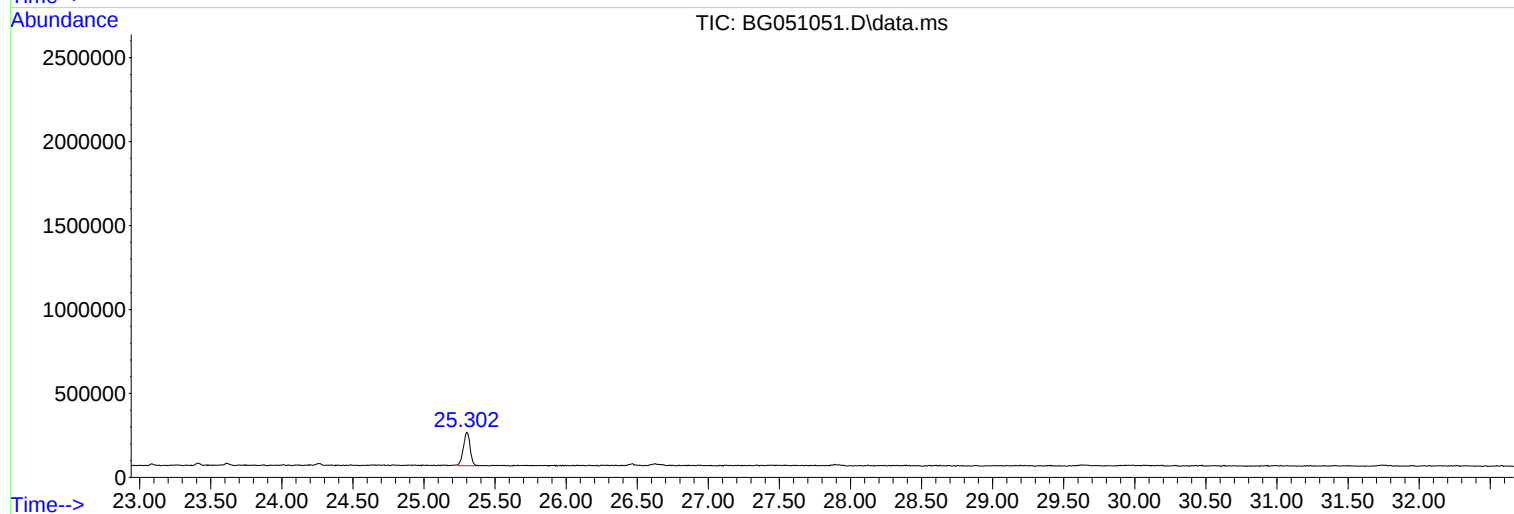
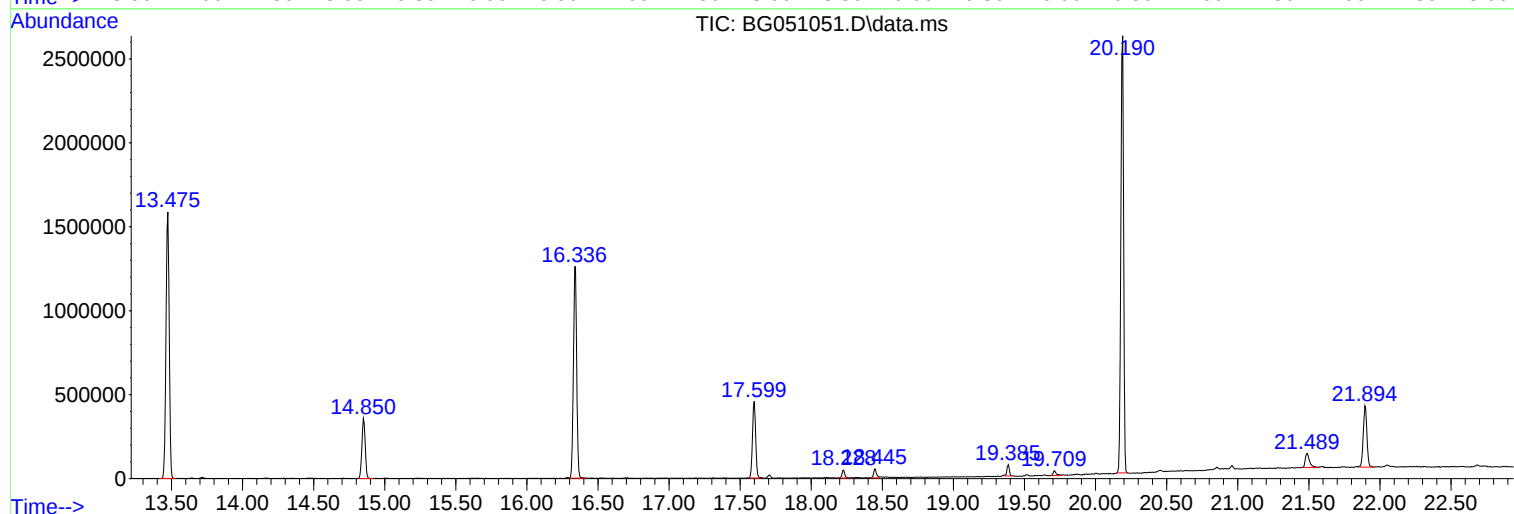
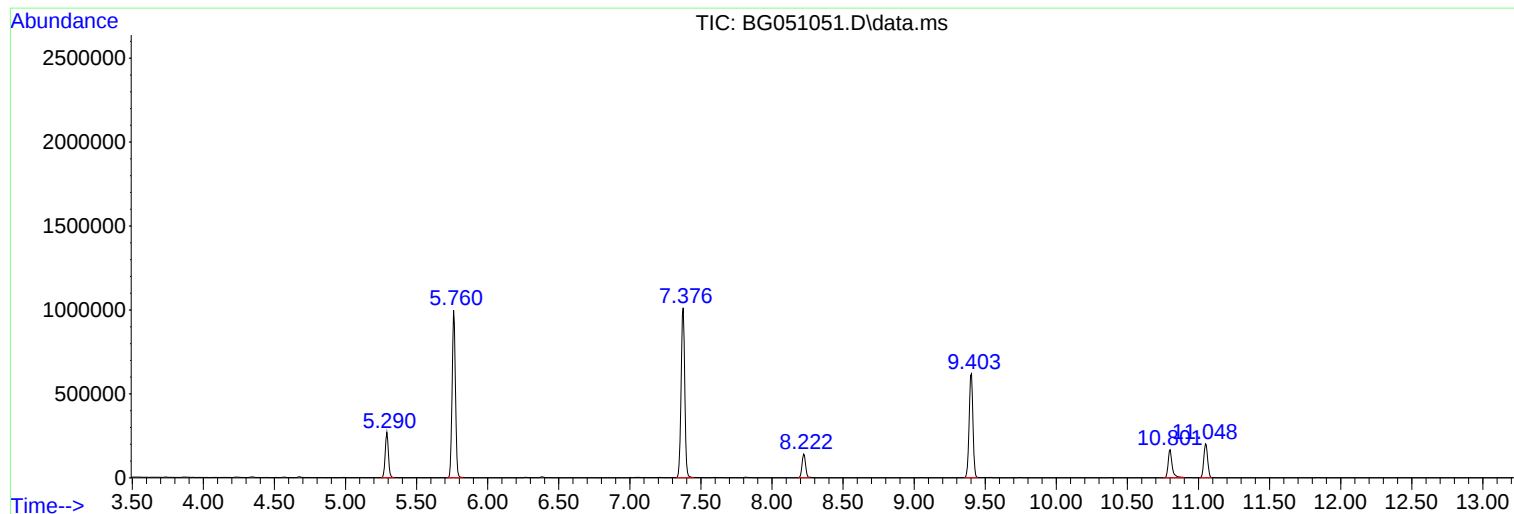
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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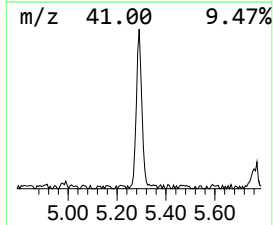
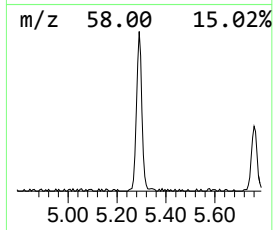
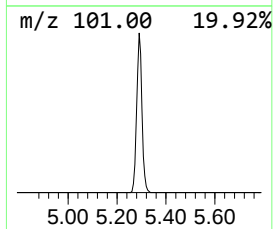
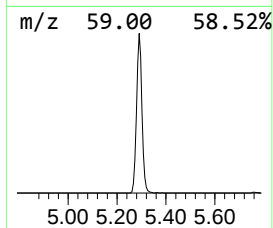
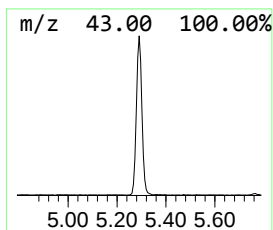
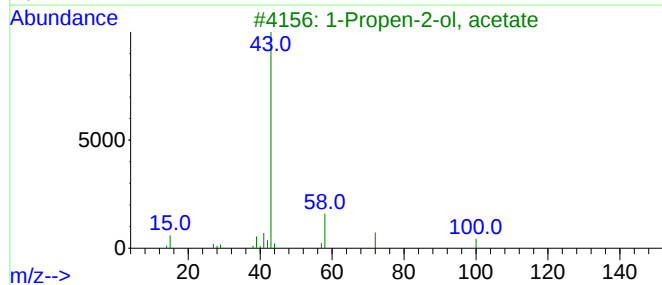
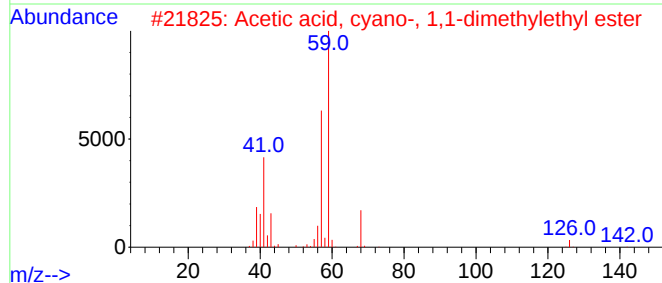
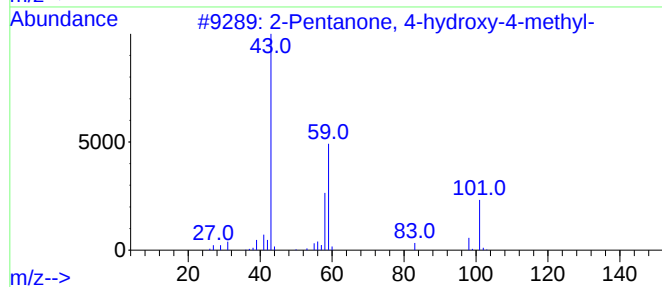
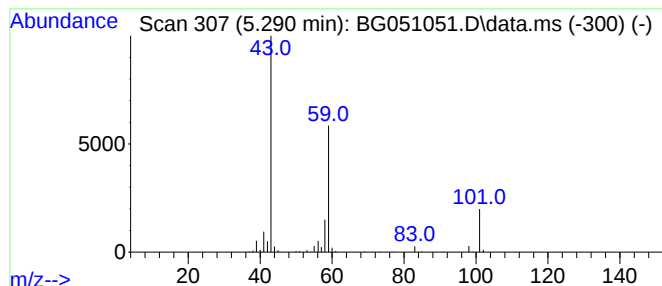
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.290	34.04 ng	418555	1,4-Dichlorobenzene-d4	8.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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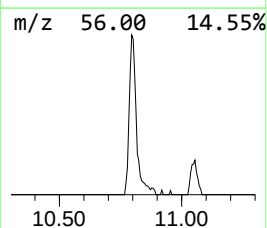
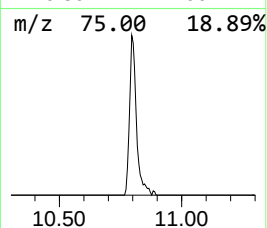
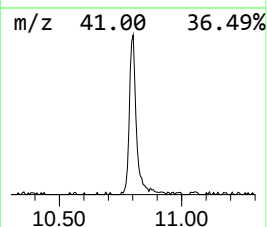
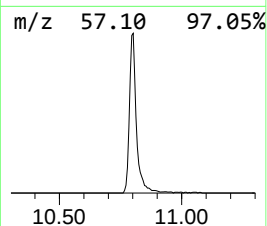
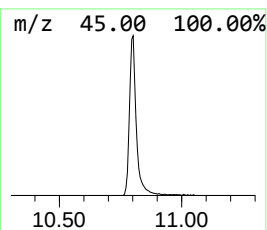
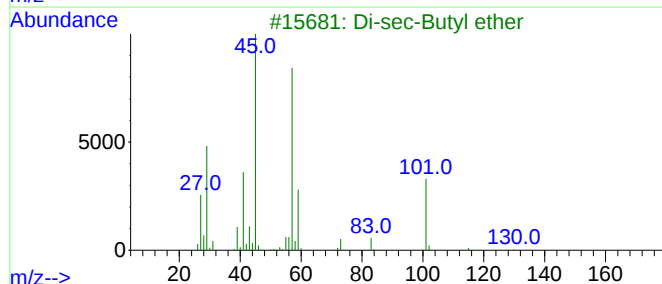
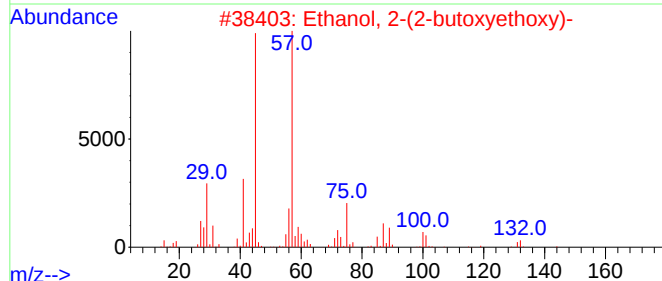
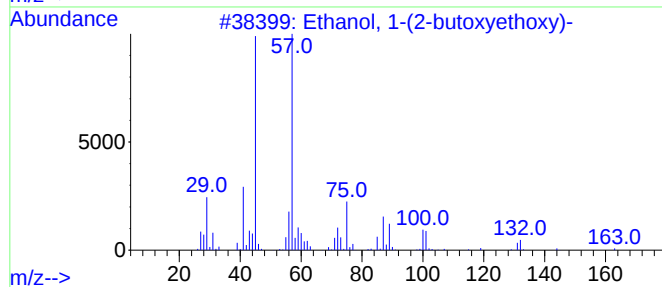
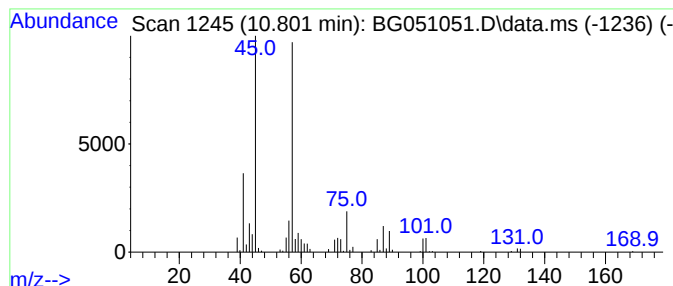
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Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.801	17.47 ng	330478	Naphthalene-d8	11.048

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	53
5			Butane, 1,1'-[ethylidenebis(oxy)]...	174	C10H22O2	000871-22-7	50



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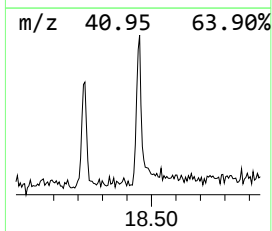
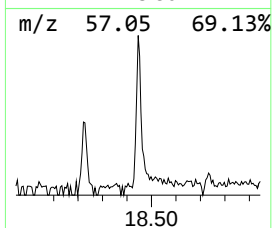
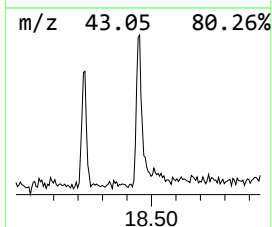
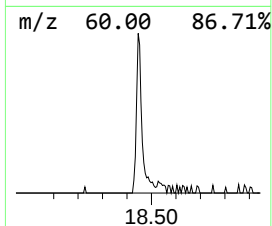
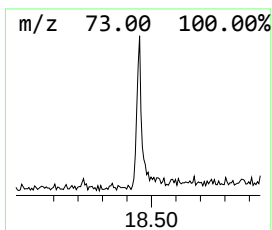
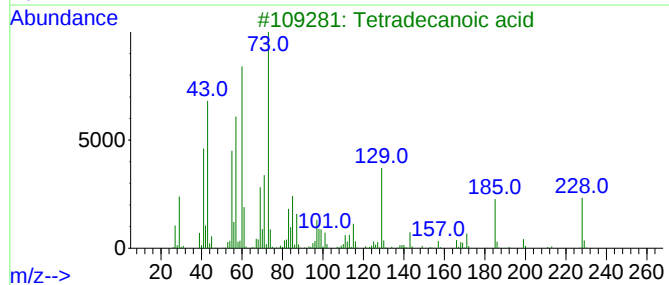
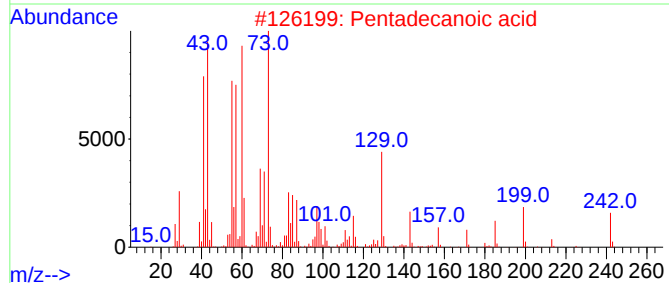
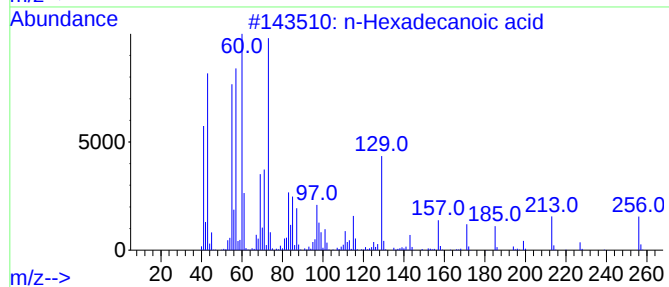
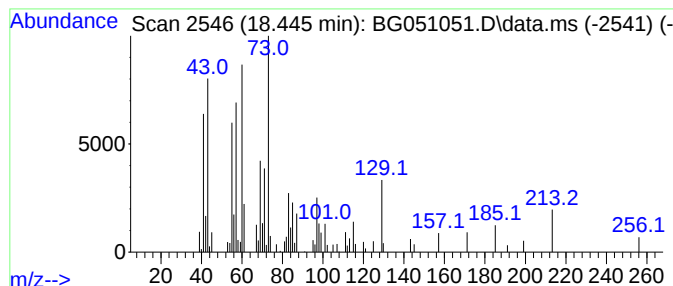
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.445	2.18 ng	76745	Phenanthrene-d10	17.599

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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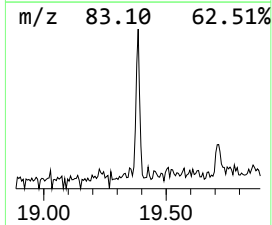
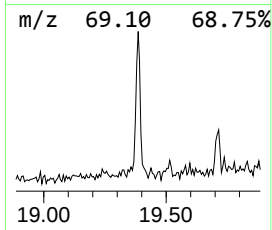
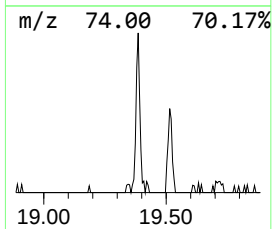
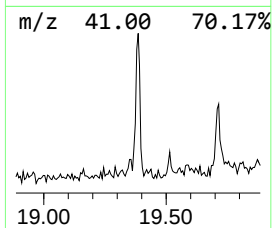
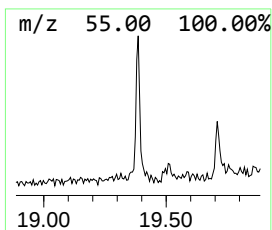
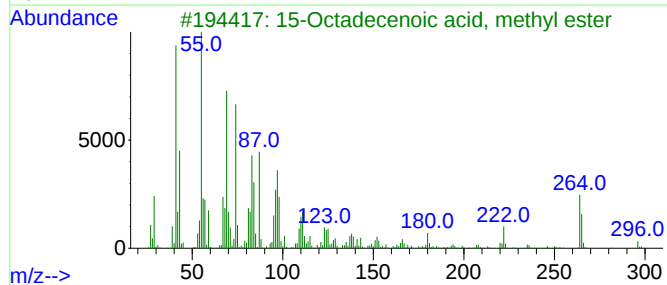
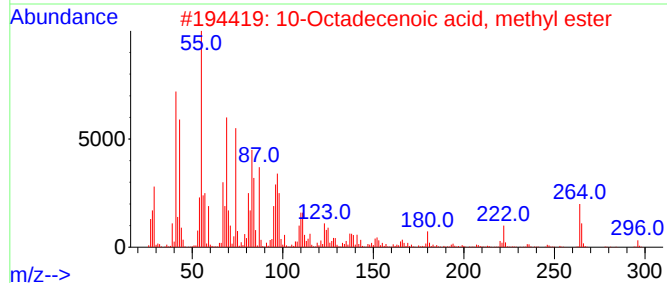
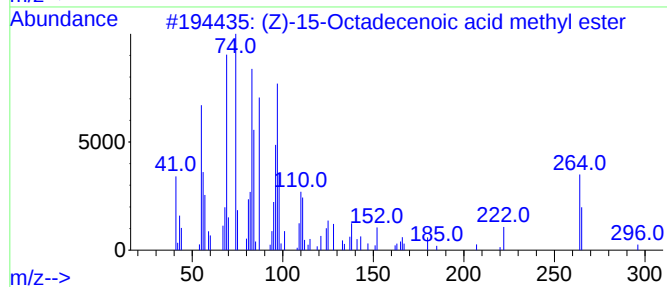
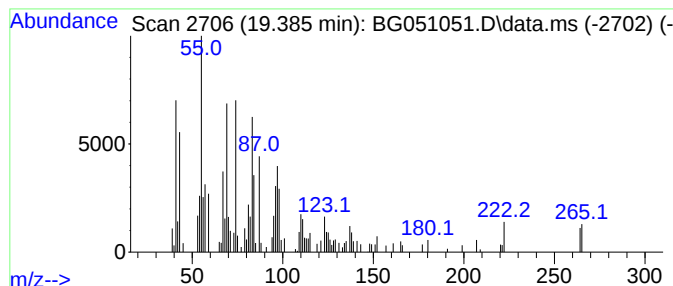
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 (Z)-15-Octadecenoic acid me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.385	2.19 ng	77024	Phenanthrene-d10	17.599	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	93
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	87
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	86



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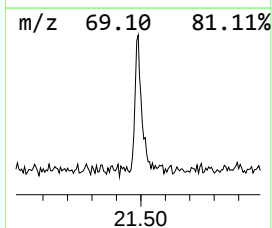
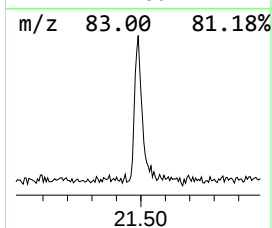
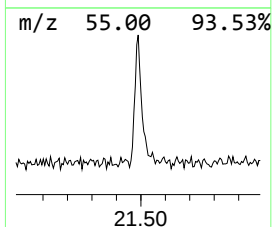
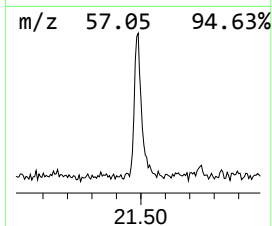
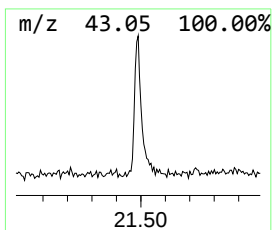
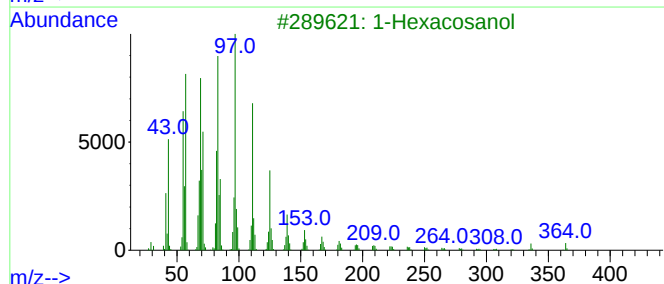
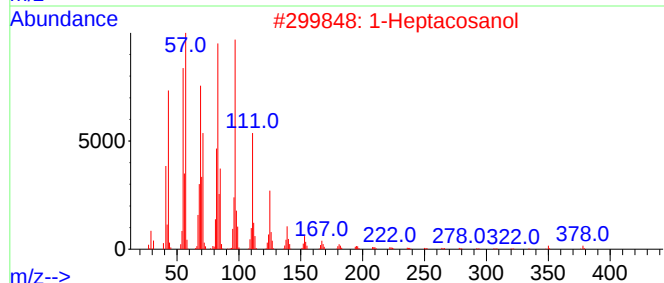
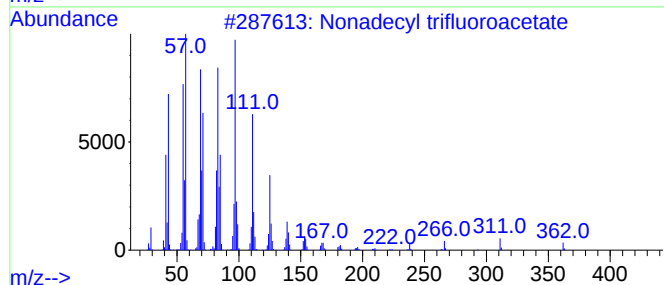
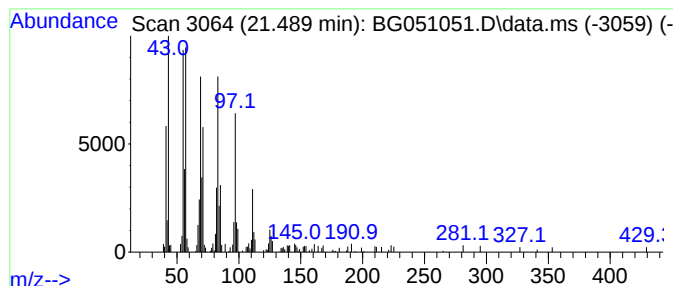
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Nonadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.489	5.25 ng	169674	Chrysene-d12	21.894

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
2			1-Heptacosanol	396	C27H56O	002004-39-9	91
3			1-Hexacosanol	382	C26H54O	000506-52-5	91
4			Octacosanol	410	C28H58O	000557-61-9	91
5			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.290	34.0	ng	418555	1	8.222	245940	20.0
Ethanol, 1-(2-b...	10.801	17.5	ng	330478	2	11.048	378331	20.0
n-Hexadecanoic ...	18.445	2.2	ng	76745	4	17.599	704652	20.0
(Z)-15-Octadece...	19.385	2.2	ng	77024	4	17.599	704652	20.0
Nonadecyl trifl...	21.489	5.3	ng	169674	5	21.894	645873	20.0