

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
 Data File : BG056338.D
 Acq On : 18 Jan 2023 21:32
 Operator : CG/JU
 Sample : 01184-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 APNB-BOT-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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056338.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.317	3	5	19	rVB	129675	170839	5.95%	1.451%
2	5.344	343	350	357	rBB2	109805	166894	5.82%	1.417%
3	5.825	424	432	442	rBV	454675	728165	25.38%	6.183%
4	7.441	700	707	718	rBV	457190	792271	27.61%	6.728%
5	8.305	847	854	863	rBB	128332	209966	7.32%	1.783%
6	9.480	1046	1054	1063	rBB	266954	473061	16.49%	4.017%
7	11.137	1328	1336	1345	rBB	162017	297528	10.37%	2.526%
8	13.546	1739	1746	1753	rBV	1076787	1614464	56.26%	13.709%
9	14.921	1970	1980	1987	rBB	325645	510903	17.81%	4.338%
10	16.254	2201	2207	2214	rBV	47248	64577	2.25%	0.548%
11	16.395	2224	2231	2243	rBV	793494	1205643	42.02%	10.238%
12	17.653	2439	2445	2452	rBV	469117	703592	24.52%	5.975%
13	18.499	2584	2589	2597	rBV	99833	136856	4.77%	1.162%
14	19.756	2798	2803	2812	rBV5	30996	48264	1.68%	0.410%
15	20.232	2877	2884	2889	rBV	2222747	2869418	100.00%	24.366%
16	21.525	3100	3104	3114	rBV2	112031	175104	6.10%	1.487%
17	21.942	3168	3175	3182	rBV2	449958	793464	27.65%	6.738%
18	25.379	3750	3760	3774	rVB2	268709	815372	28.42%	6.924%

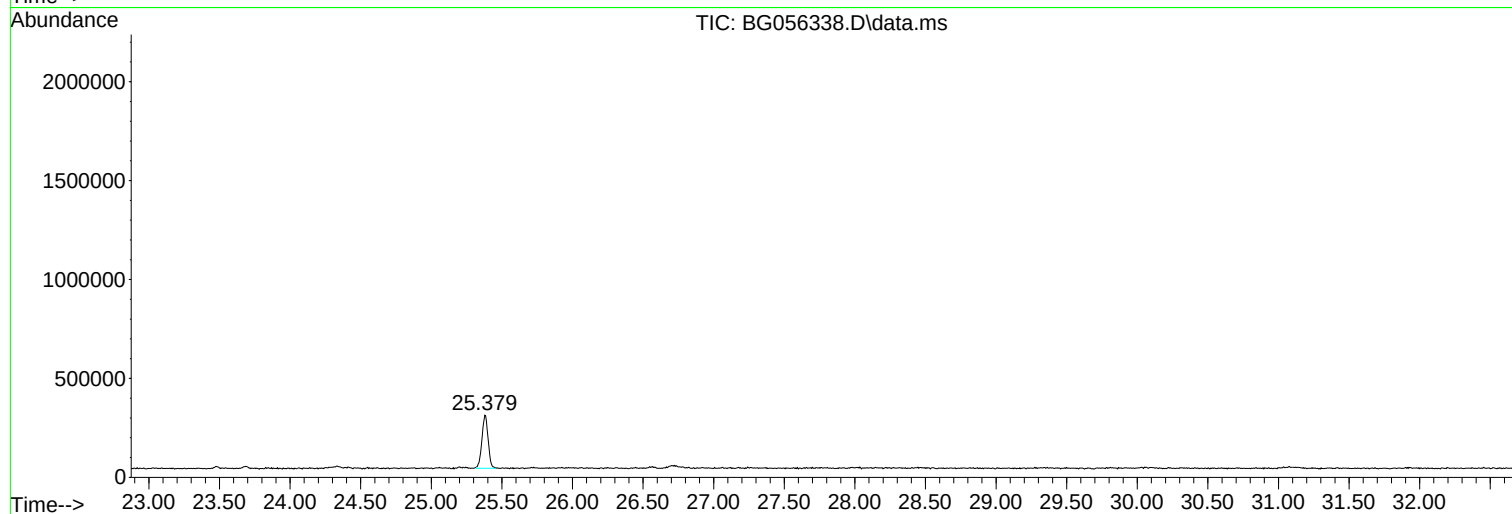
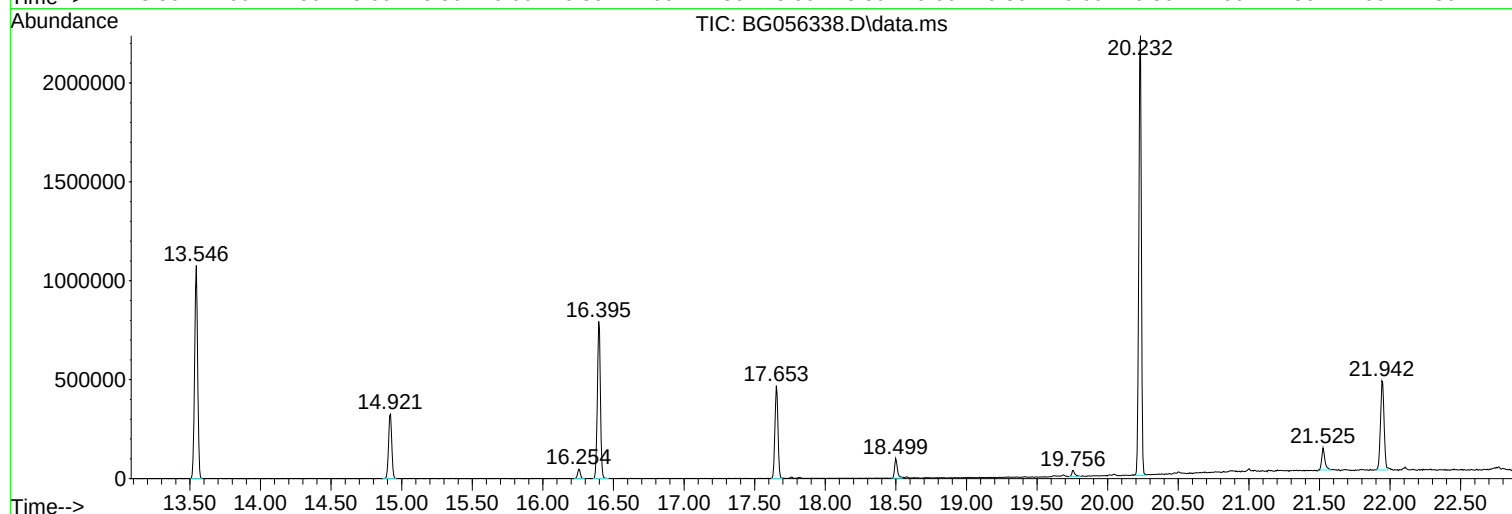
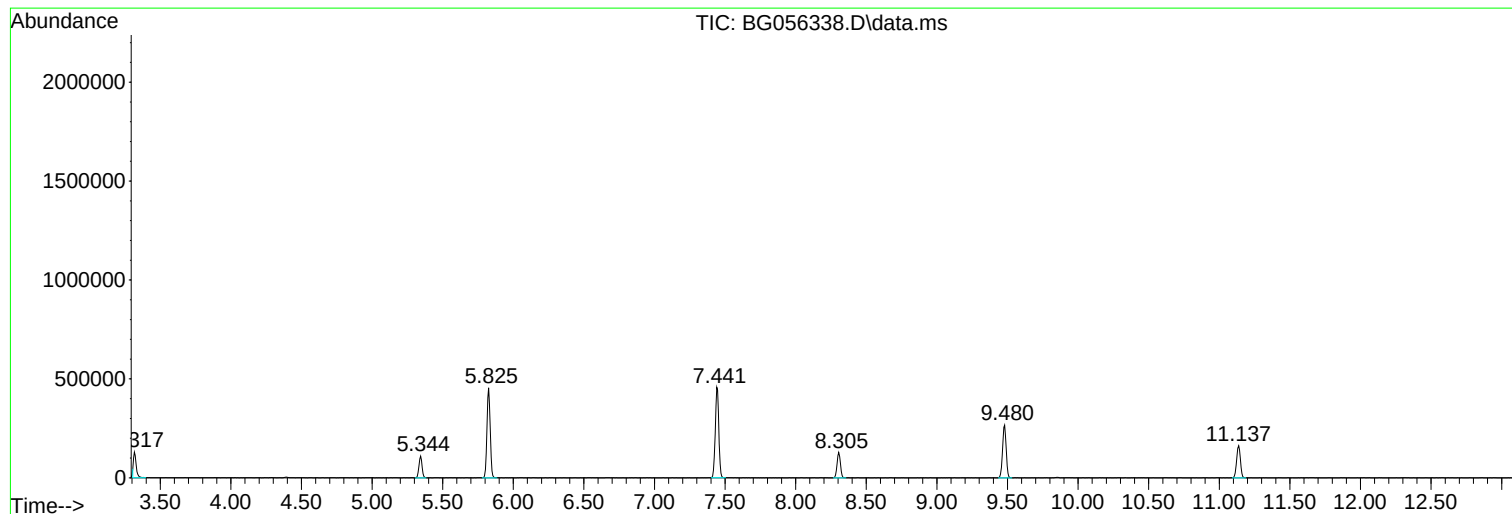
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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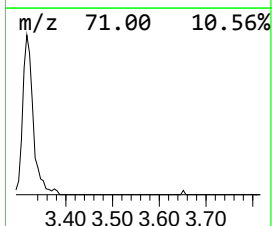
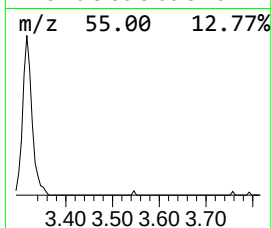
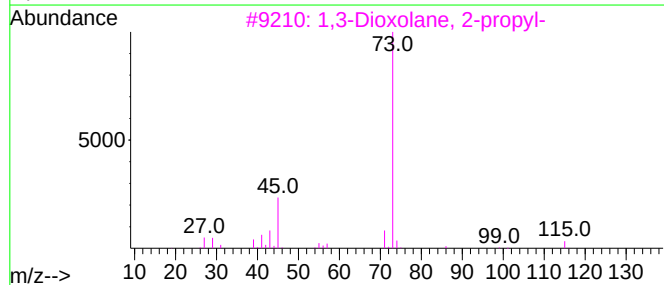
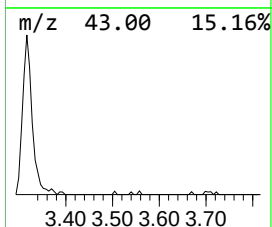
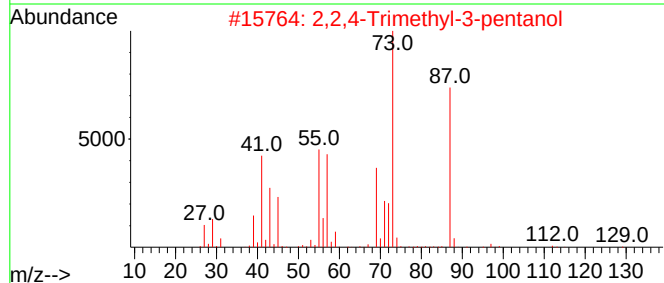
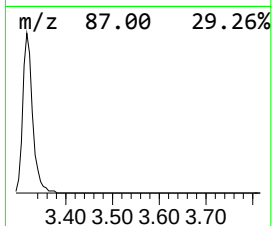
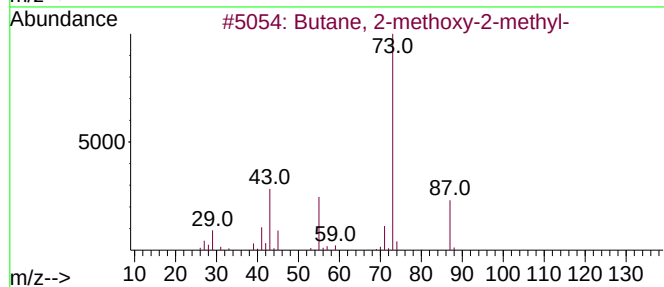
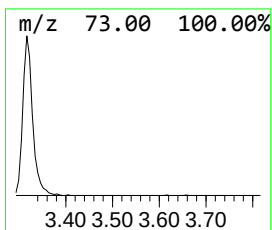
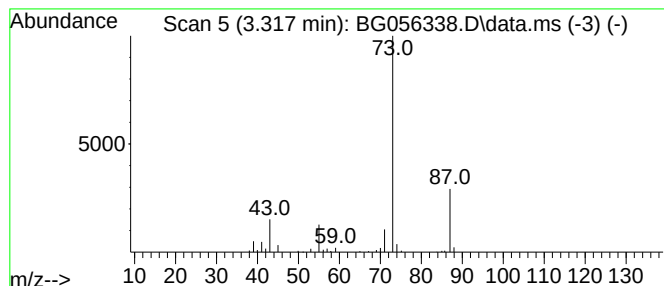
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.317	16.27 ng	170839	1,4-Dichlorobenzene-d4	8.305

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5			2-Propanone, oxime	73	C3H7NO	000127-06-0	7



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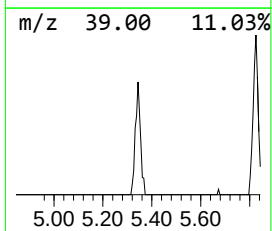
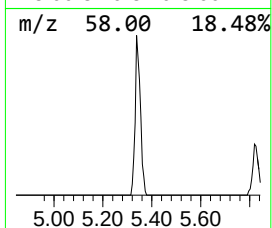
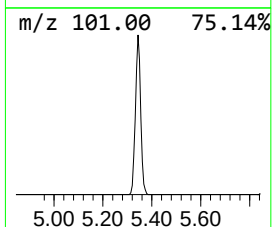
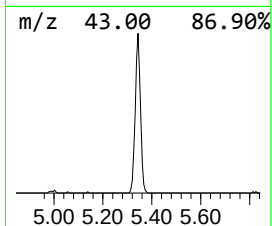
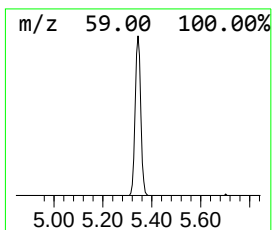
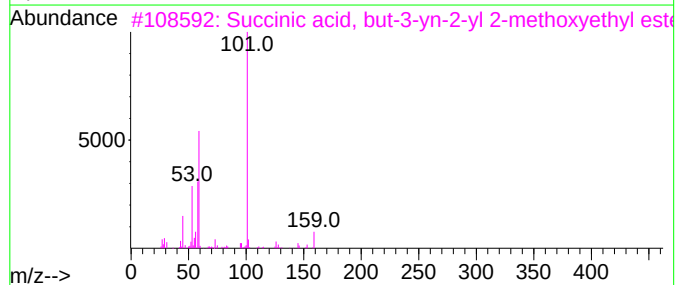
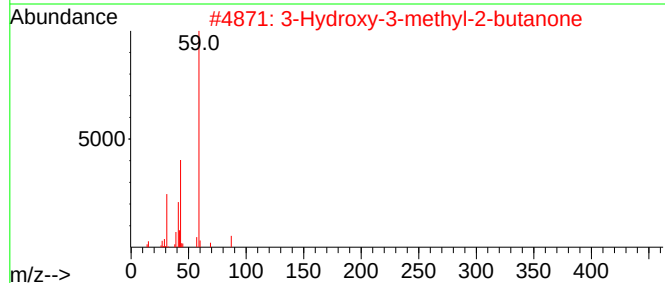
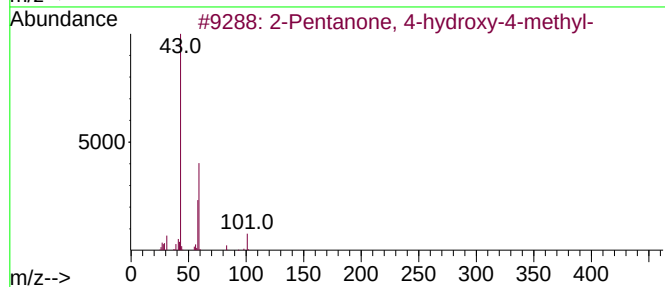
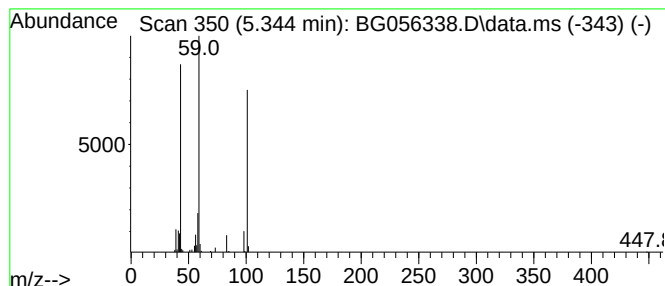
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.344	15.90 ng	166894	1,4-Dichlorobenzene-d4	8.305

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
3			Succinic acid, but-3-yn-2-yl 2-m...	228	C11H16O5	1000390-73-3	23
4			1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	17
5			Succinic acid, 2-chloropropyl he...	278	C13H23ClO4	1000349-37-3	16



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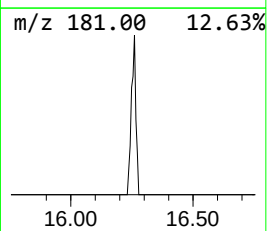
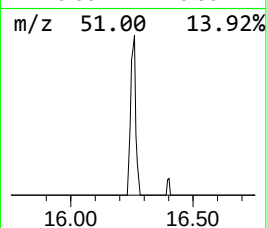
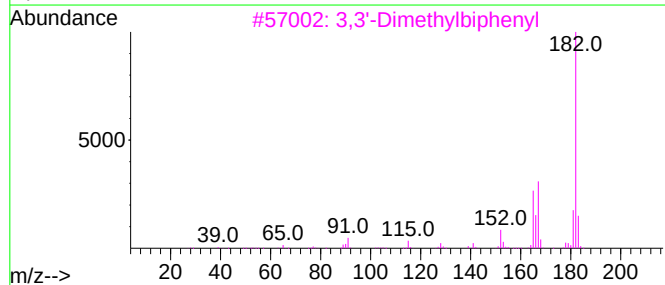
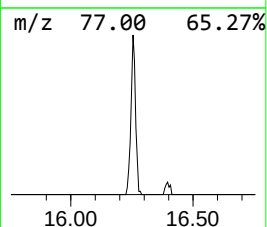
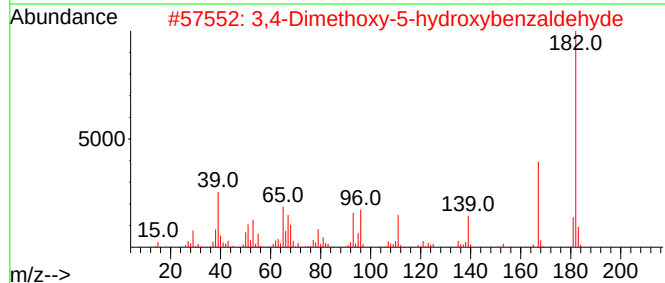
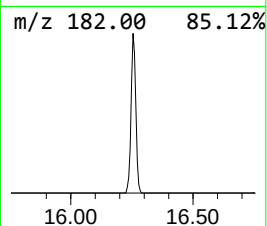
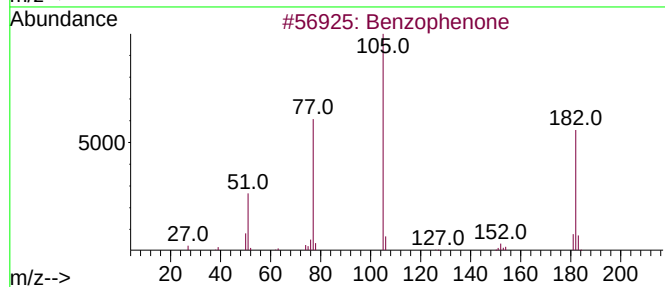
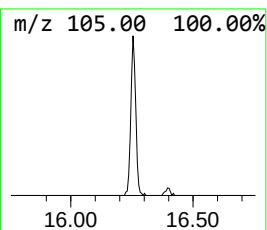
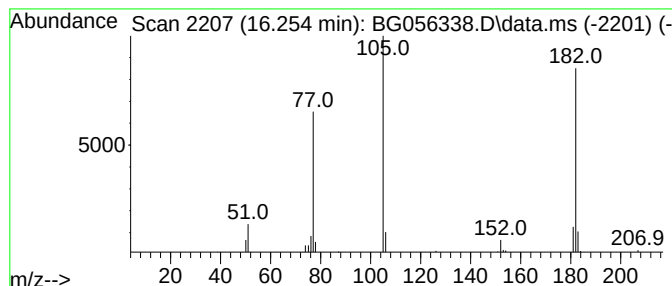
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.254	2.53 ng	64577	Acenaphthene-d10	14.921

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	91
2			3,4-Dimethoxy-5-hydroxybenzaldehyde	182	C9H10O4	029865-90-5	46
3			3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43
4			1-Methyl-1,6-diazaplenalene	182	C12H10N2	079691-99-9	38
5			1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	35



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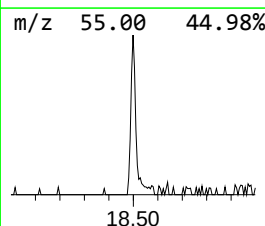
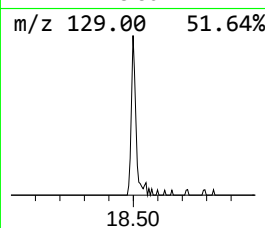
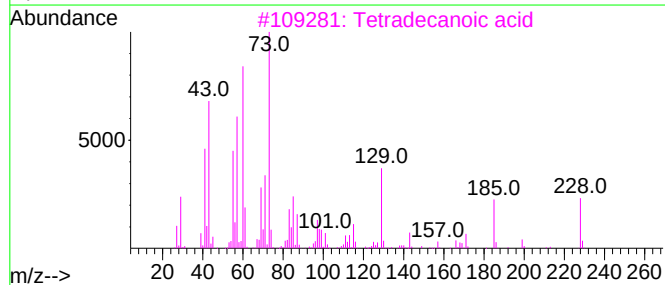
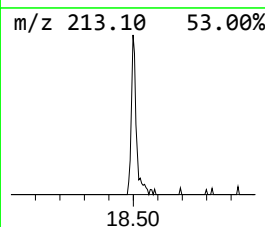
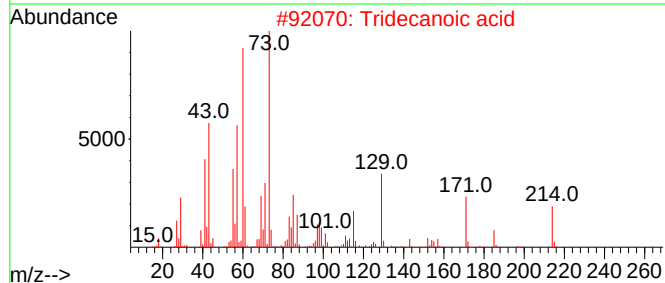
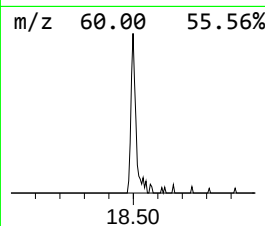
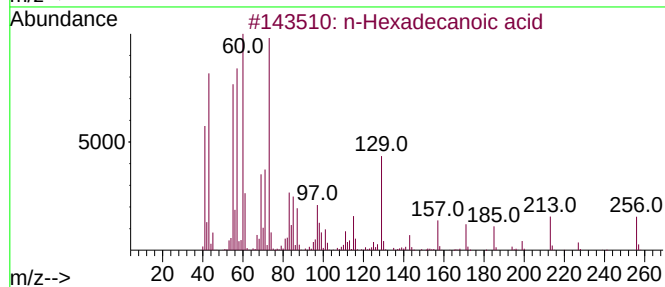
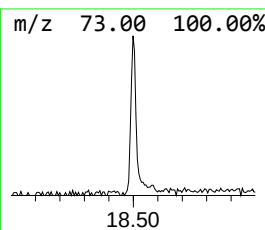
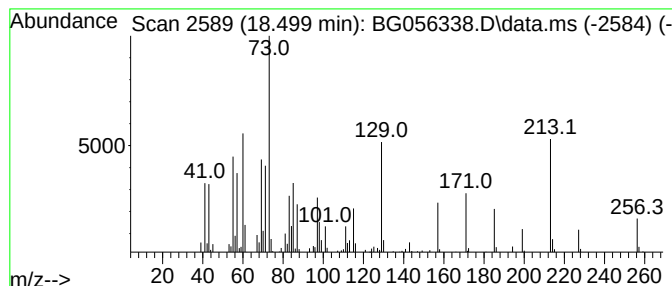
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.499	3.89 ng	136856	Phenanthrene-d10	17.653

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Dodecanoic acid	200	C12H24O2	000143-07-7	58
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	43



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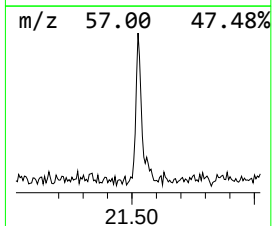
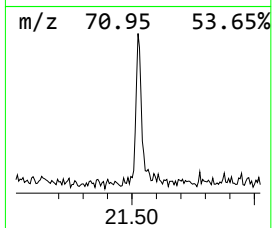
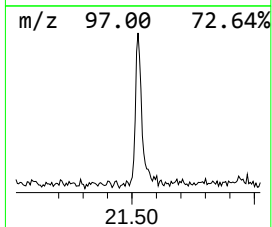
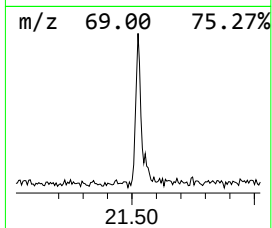
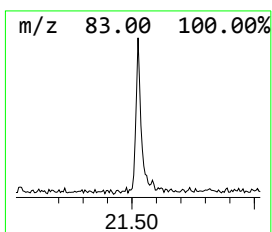
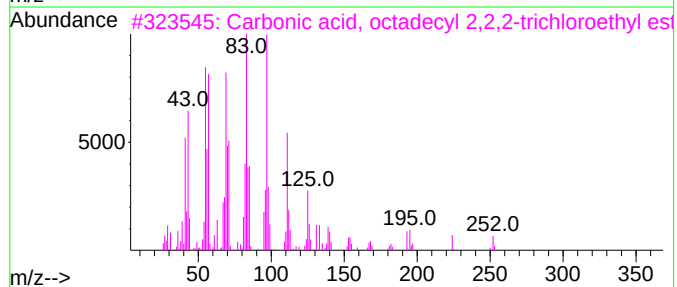
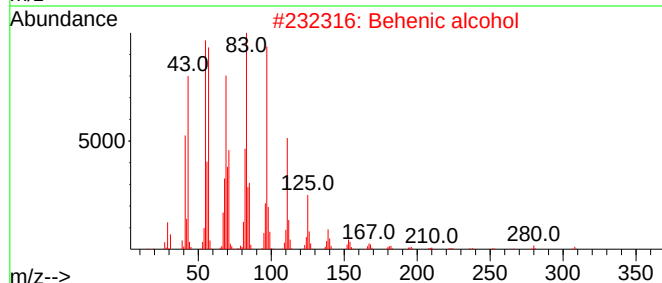
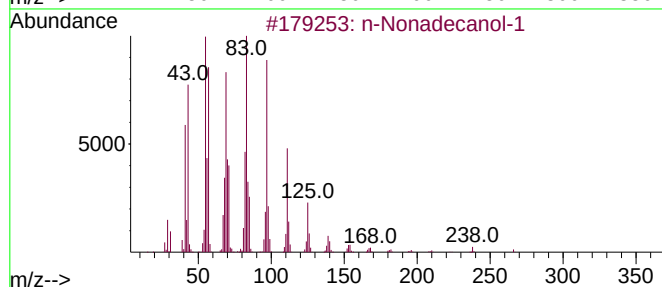
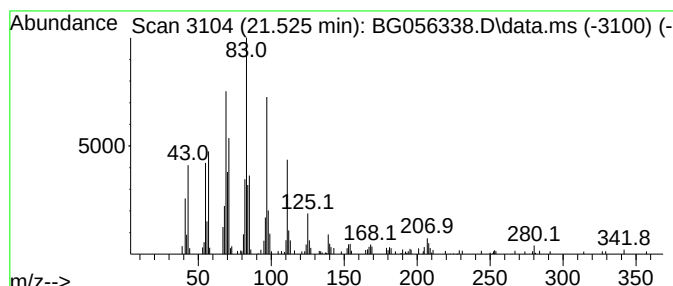
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.525	4.41 ng	175104	Chrysene-d12	21.942

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	80
2		Behenic alcohol	326	C22H46O	000661-19-8	78
3		Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	64
4		1-Hexacosanol	382	C26H54O	000506-52-5	43
5		Carbonic acid, pentadecyl 2,2,2-...	402	C18H33Cl3O3	1000314-56-1	38



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.317	16.3	ng	170839	1	8.305	209966	20.0
2-Pentanone, 4-...	5.344	15.9	ng	166894	1	8.305	209966	20.0
Benzophenone	16.254	2.5	ng	64577	3	14.921	510903	20.0
n-Hexadecanoic ...	18.499	3.9	ng	136856	4	17.653	703592	20.0
n-Nonadecanol-1	21.525	4.4	ng	175104	5	21.942	793464	20.0