

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
 Data File : BG055554.D
 Acq On : 11 Nov 2022 1:06
 Operator : CG/JU
 Sample : N5476-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RED-006-5

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055554.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.332	3	7	26	rVB	695446	1174136	34.08%	7.567%
2	4.713	235	242	249	rBV	32927	52180	1.51%	0.336%
3	5.324	340	346	354	rBV	67615	104452	3.03%	0.673%
4	5.794	419	426	435	rBV	441276	696953	20.23%	4.492%
5	7.398	690	699	707	rBV	270733	458671	13.31%	2.956%
6	8.268	840	847	854	rBV	164864	273509	7.94%	1.763%
7	9.437	1036	1046	1055	rBV	598403	1059122	30.74%	6.826%
8	11.094	1318	1328	1337	rBV	220872	399860	11.61%	2.577%
9	13.514	1733	1740	1747	rBV	1542984	2413101	70.04%	15.552%
10	14.883	1966	1973	1980	rVB	357840	555334	16.12%	3.579%
11	16.364	2218	2225	2236	rBV	1343187	2003394	58.15%	12.912%
12	17.621	2433	2439	2446	rBV	463815	728839	21.16%	4.697%
13	18.485	2581	2586	2598	rBV	84372	146027	4.24%	0.941%
14	19.748	2796	2801	2807	rBV3	42866	64035	1.86%	0.413%
15	20.212	2874	2880	2886	rBV	2675340	3445108	100.00%	22.203%
16	21.528	3099	3104	3115	rBV	112783	192035	5.57%	1.238%
17	21.922	3164	3171	3182	rVB	496611	846013	24.56%	5.452%
18	23.708	3471	3475	3481	rVB4	26114	51384	1.49%	0.331%
19	25.342	3743	3753	3768	rVB2	284476	852069	24.73%	5.491%

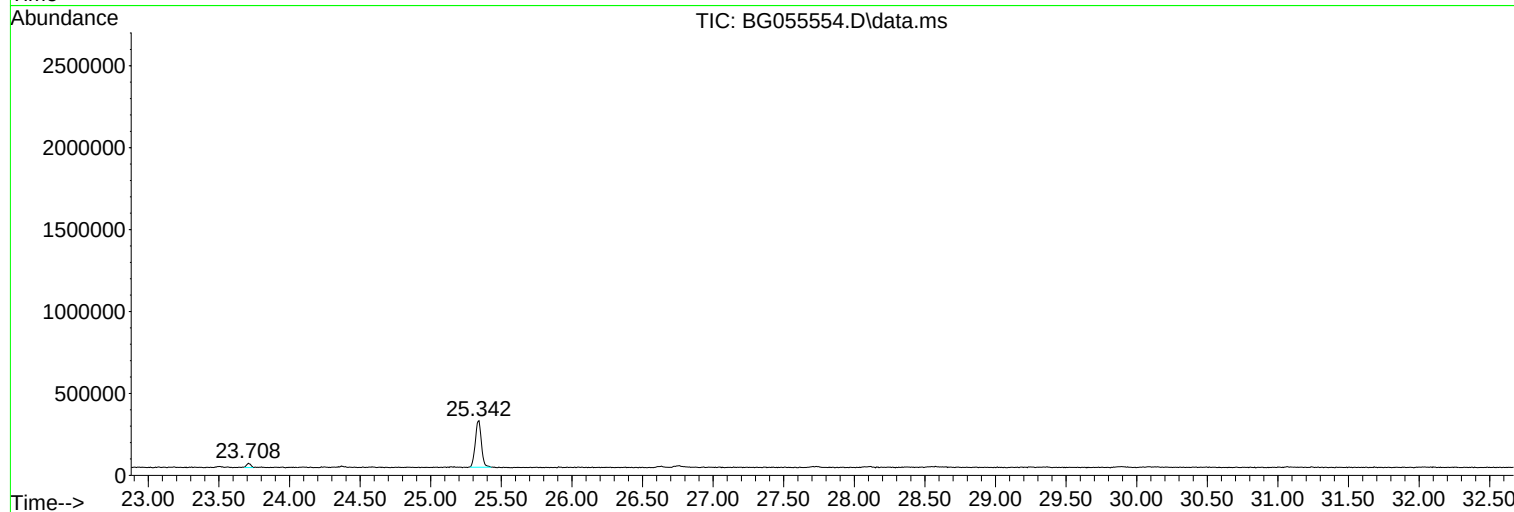
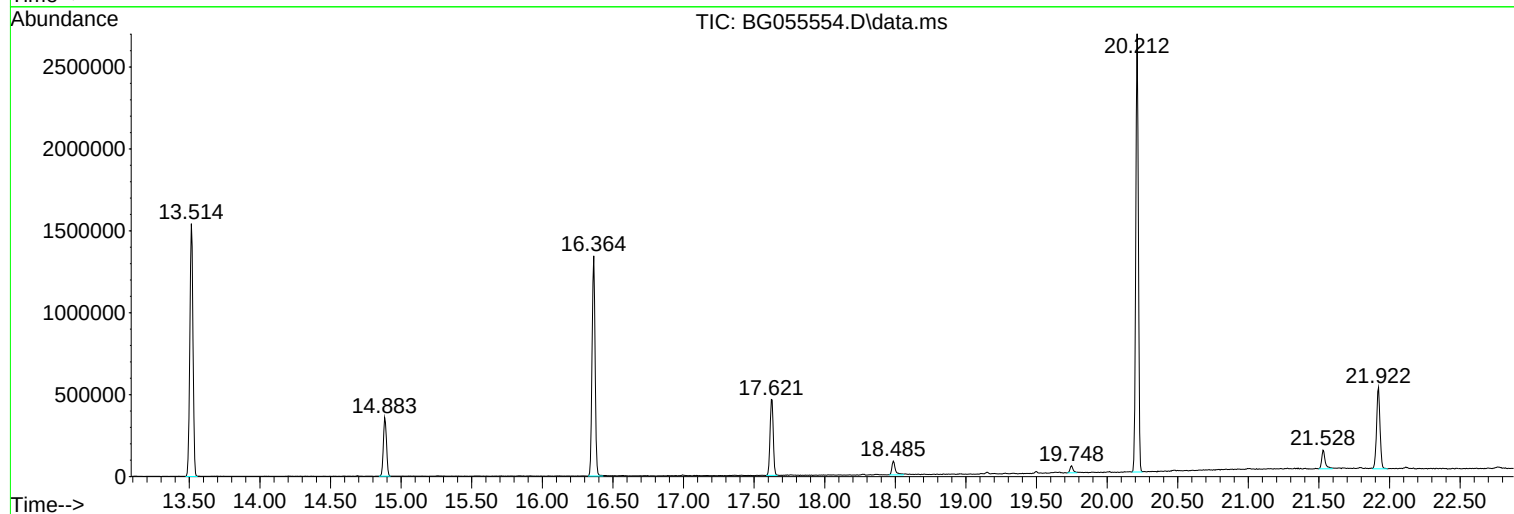
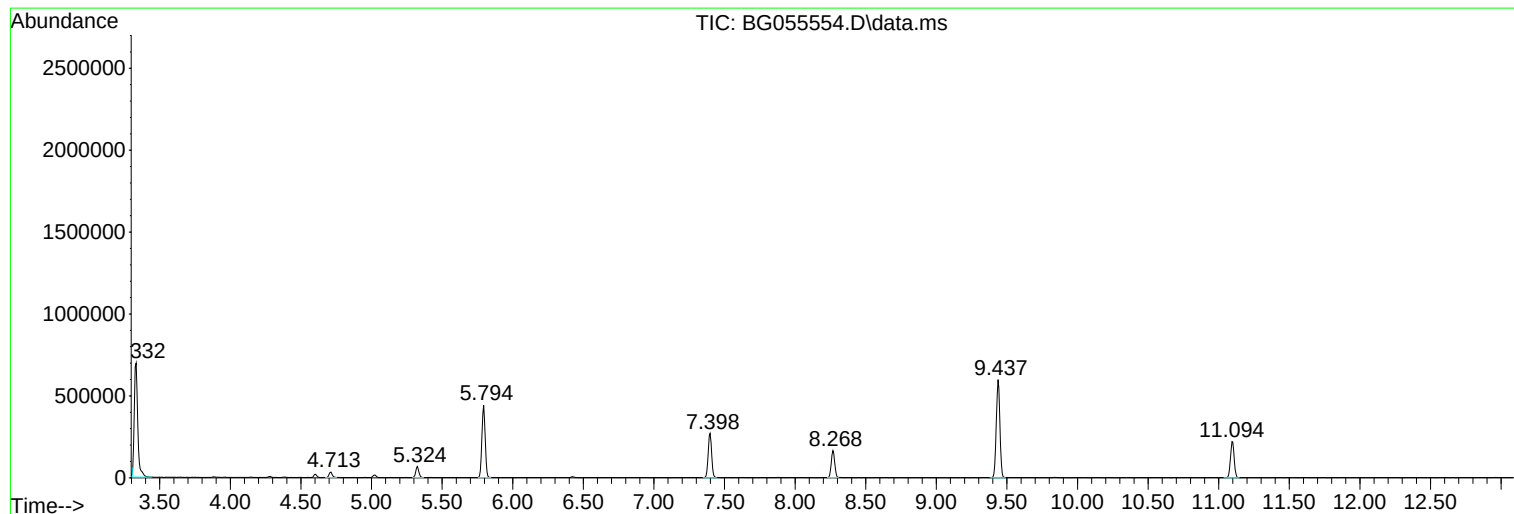
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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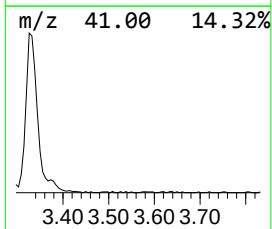
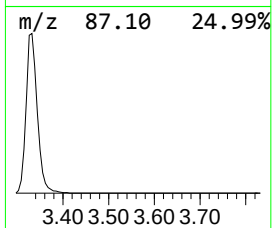
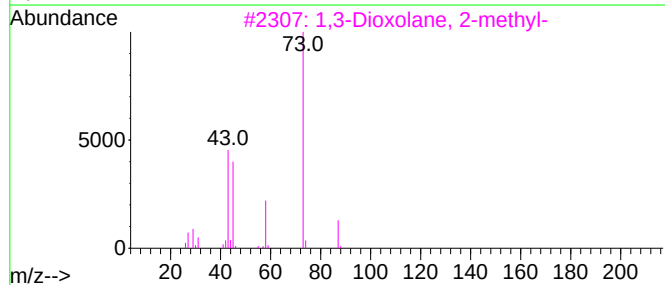
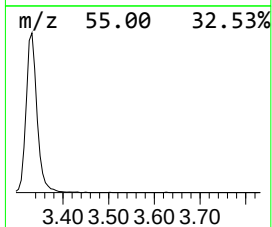
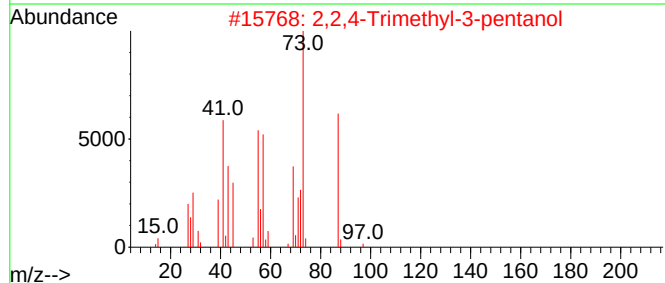
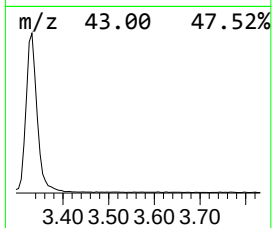
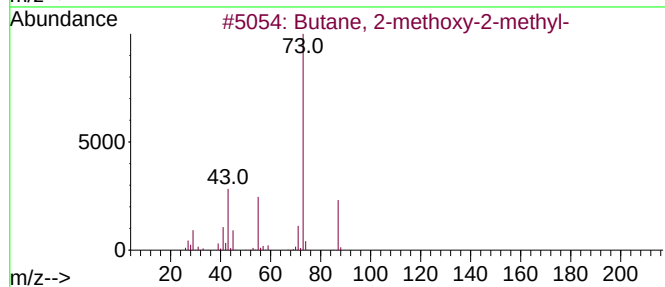
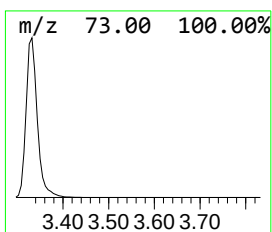
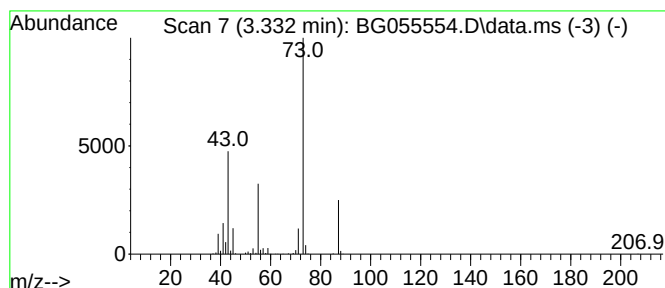
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.332	85.86 ng	1174140	1,4-Dichlorobenzene-d4	8.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	17



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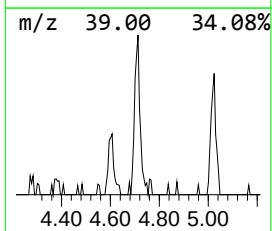
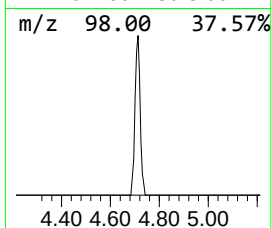
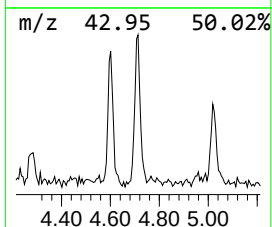
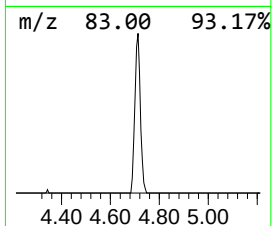
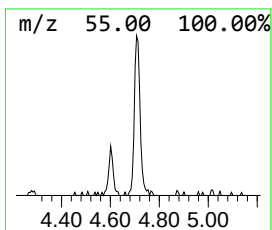
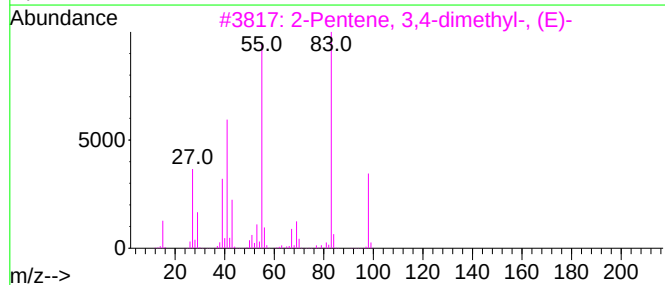
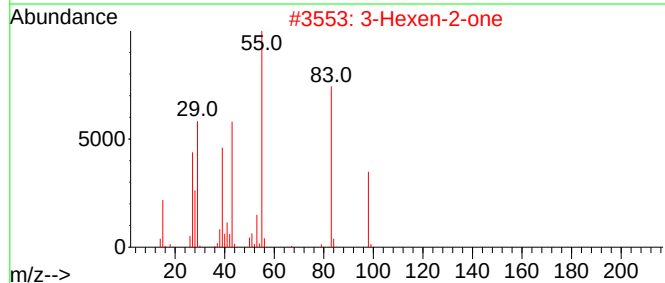
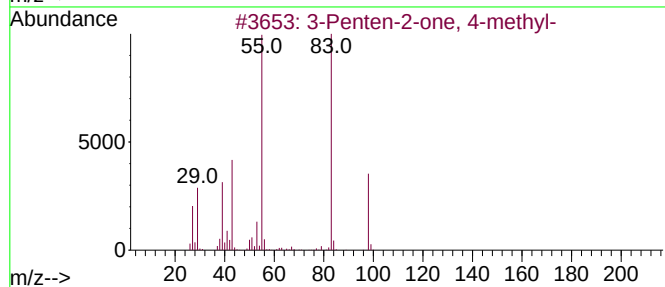
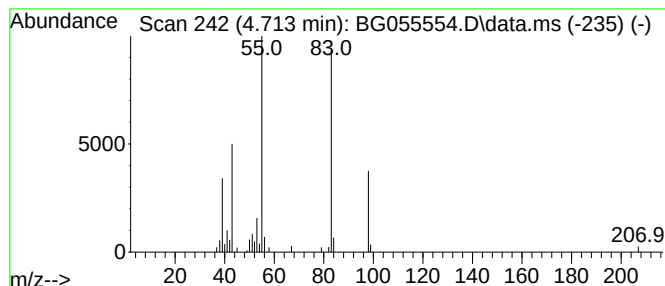
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.713	3.82 ng	52180	1,4-Dichlorobenzene-d4	8.268

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	87
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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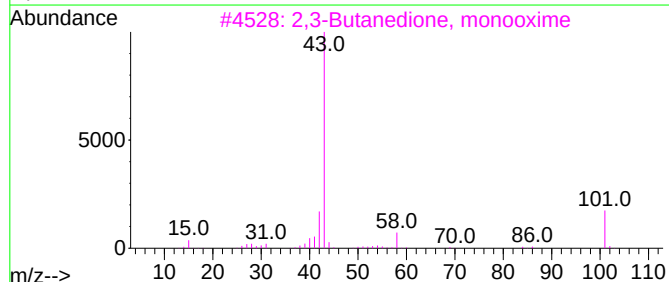
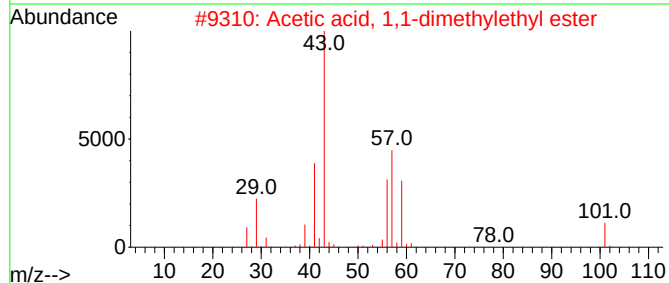
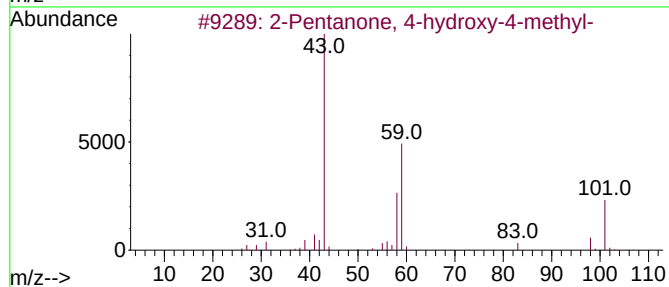
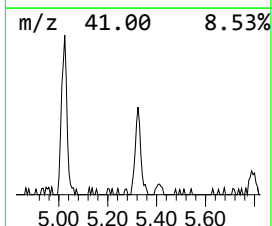
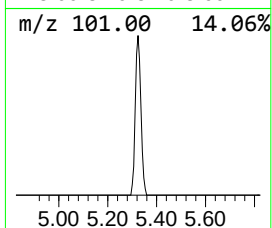
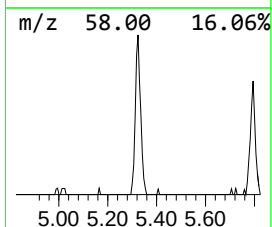
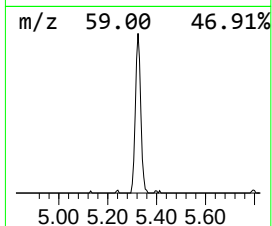
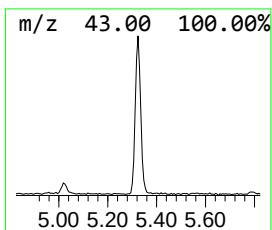
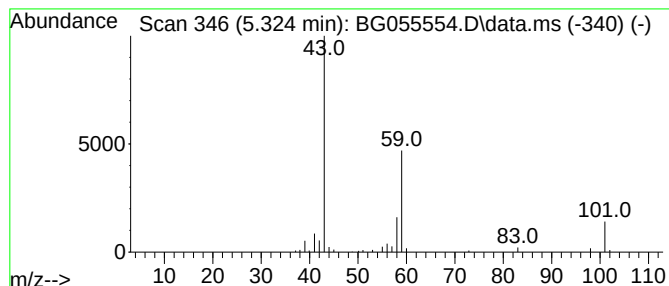
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.324	7.64 ng	104452	1,4-Dichlorobenzene-d4	8.268

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Acetone	58	C3H6O	000067-64-1	12



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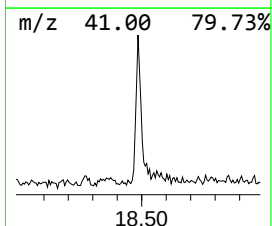
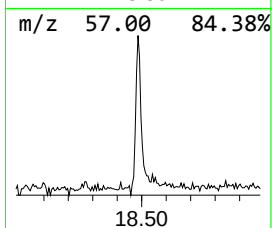
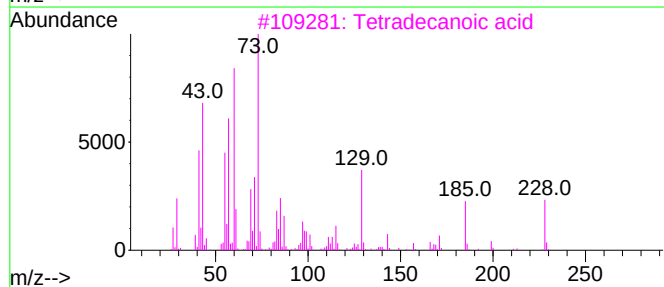
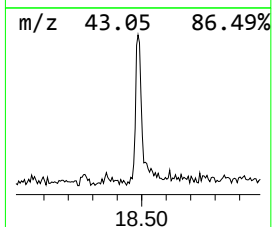
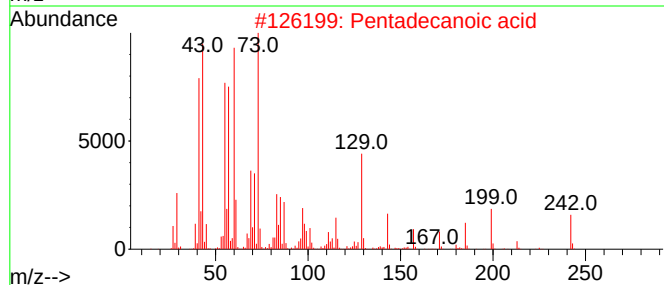
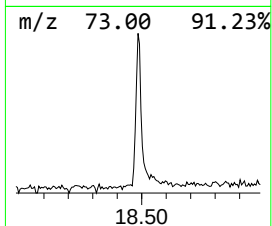
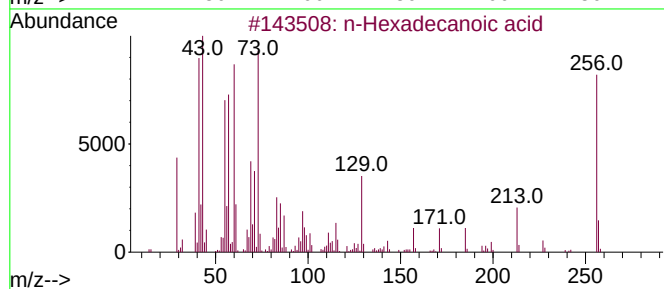
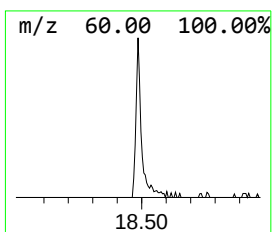
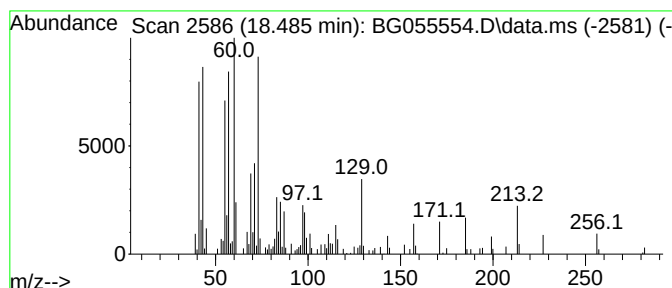
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.485	4.01 ng	146027	Phenanthrene-d10	17.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Dodecanoic acid	200	C12H24O2	000143-07-7	64
5			Octanoic acid	144	C8H16O2	000124-07-2	46



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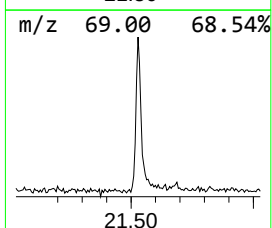
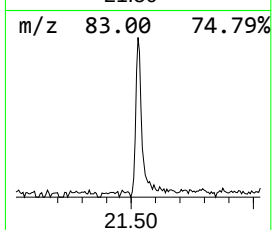
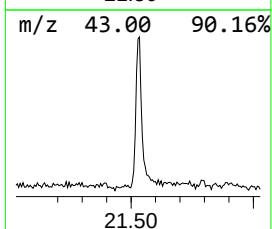
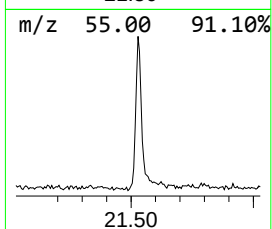
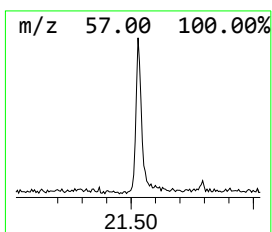
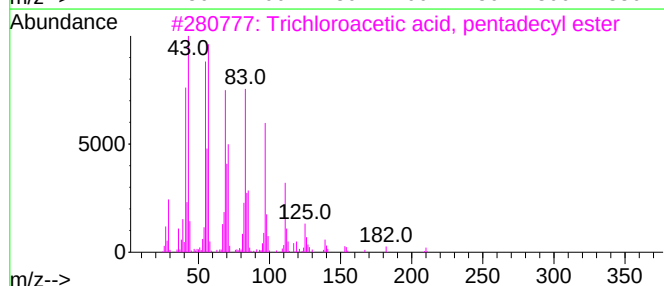
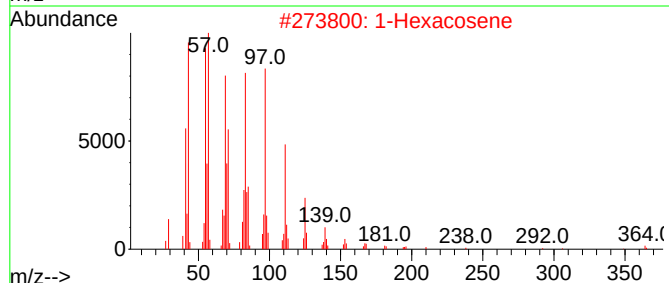
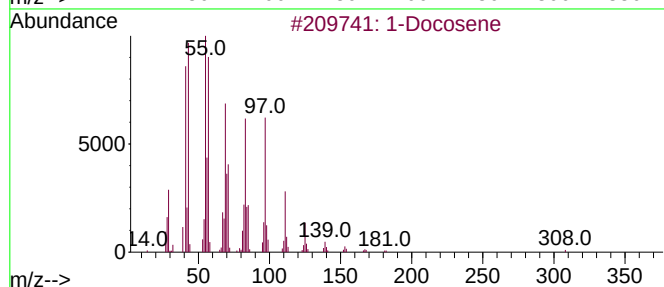
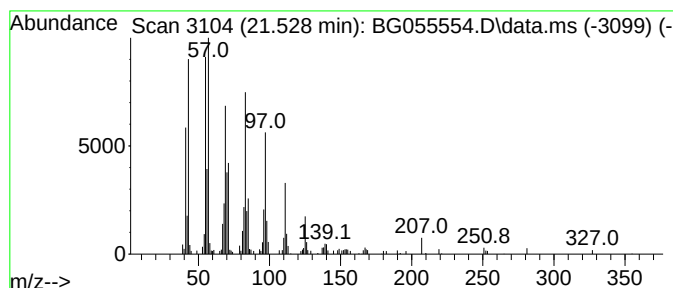
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.528	4.54 ng	192035	Chrysene-d12	21.922	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	1-Hexacosene	364	C26H52	018835-33-1	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl13O2	074339-53-0	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	Octacosanol	410	C28H58O	000557-61-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.332	85.9	ng	1174140	1	8.268	273509	20.0
3-Penten-2-one,...	4.713	3.8	ng	52180	1	8.268	273509	20.0
2-Pentanone, 4-...	5.324	7.6	ng	104452	1	8.268	273509	20.0
n-Hexadecanoic ...	18.485	4.0	ng	146027	4	17.627	728839	20.0
1-Docosene	21.528	4.5	ng	192035	5	21.922	846013	20.0