

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
 Data File : BP007931.D
 Acq On : 10 Nov 2021 21:39
 Operator : CG/JU
 Sample : M4605-08
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 VWE-B19-110821-GW

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-BP110221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.440	359	366	375	rBV	1284701	1850034	20.70%	5.100%
2	7.028	629	636	649	rBV	729451	1162360	13.01%	3.204%
3	7.852	769	776	784	rBV	397824	644865	7.22%	1.778%
4	9.010	966	973	984	rBV	1306233	2226032	24.91%	6.136%
5	9.999	1133	1141	1148	rBV	72550	124307	1.39%	0.343%
6	10.652	1242	1252	1259	rBV	476041	801693	8.97%	2.210%
7	11.475	1383	1392	1401	rBV	93048	169971	1.90%	0.469%
8	12.304	1524	1533	1549	rBV	211075	388510	4.35%	1.071%
9	12.787	1606	1615	1623	rBV2	53333	91237	1.02%	0.251%
10	13.116	1664	1671	1685	rBV	3626214	5364016	60.02%	14.786%
11	14.493	1898	1905	1917	rBV	688242	1094728	12.25%	3.018%
12	14.940	1972	1981	1998	rBV	1332280	2289120	25.61%	6.310%
13	15.316	2038	2045	2055	rBV	267901	365032	4.08%	1.006%
14	15.987	2152	2159	2180	rBV	3173595	4865666	54.44%	13.412%
15	16.745	2283	2288	2304	rBV	129362	194975	2.18%	0.537%
16	17.245	2367	2373	2386	rBV	991321	1417998	15.87%	3.909%
17	18.139	2521	2525	2533	rBV	87526	133224	1.49%	0.367%
18	19.375	2732	2735	2743	rBV6	64672	96571	1.08%	0.266%
19	19.810	2803	2809	2817	rBV	7510437	8937651	100.00%	24.636%
20	21.339	3064	3069	3078	rBV	1459474	1924841	21.54%	5.306%
21	23.745	3472	3478	3487	rVB2	1033029	2135432	23.89%	5.886%

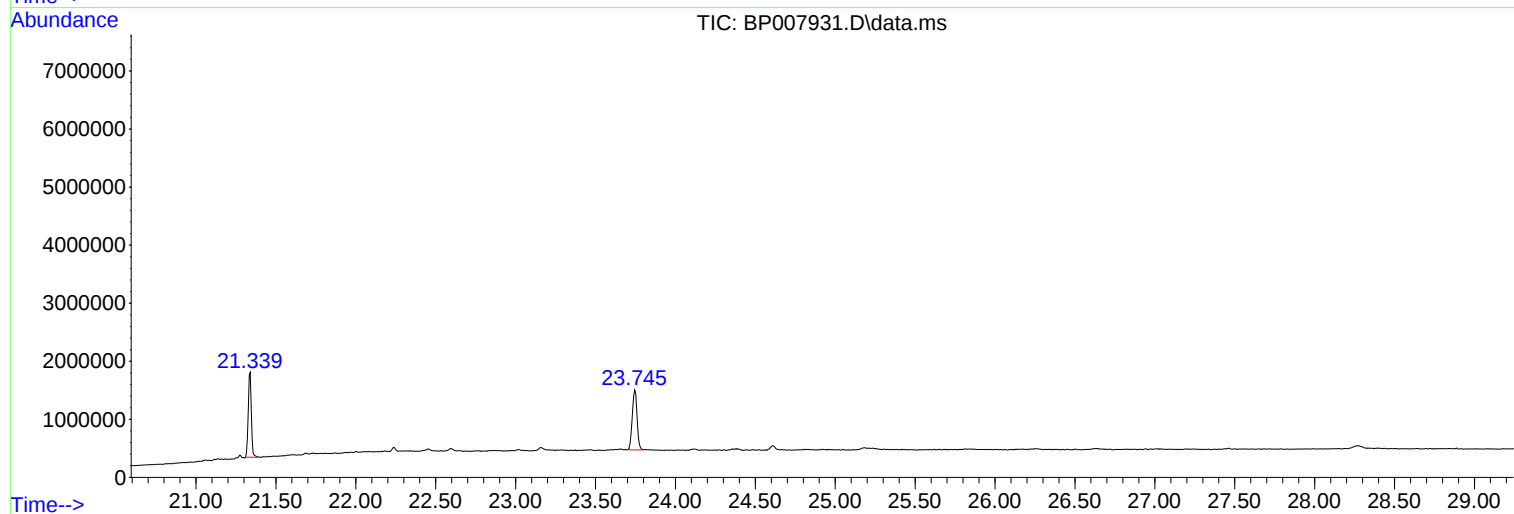
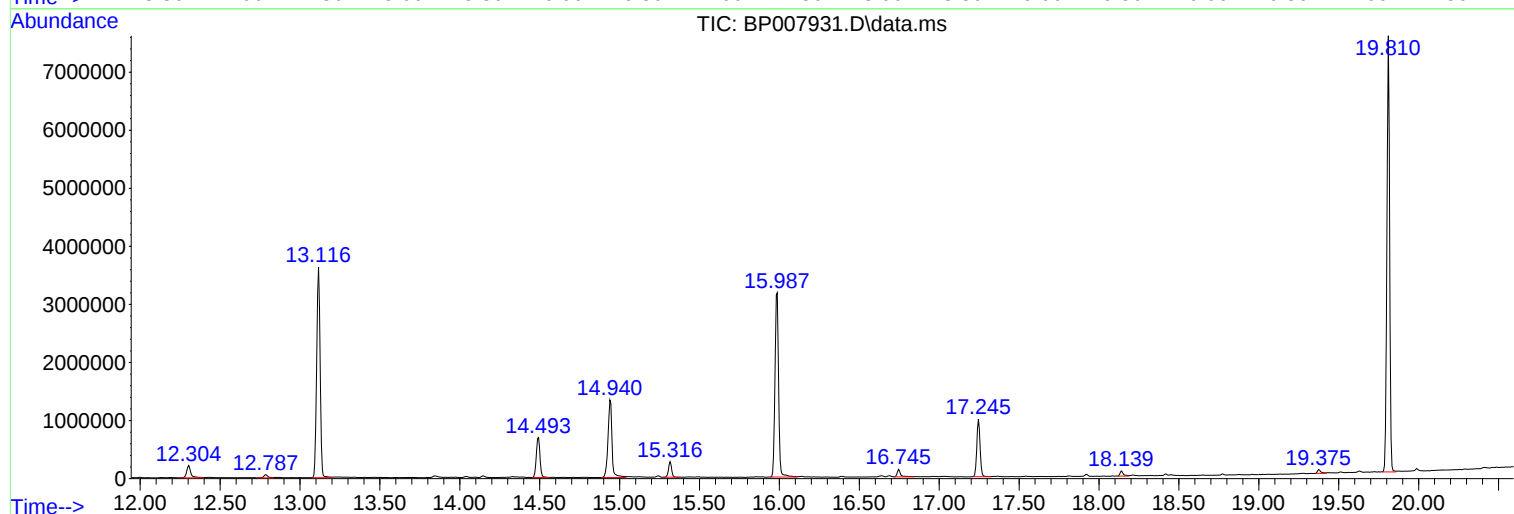
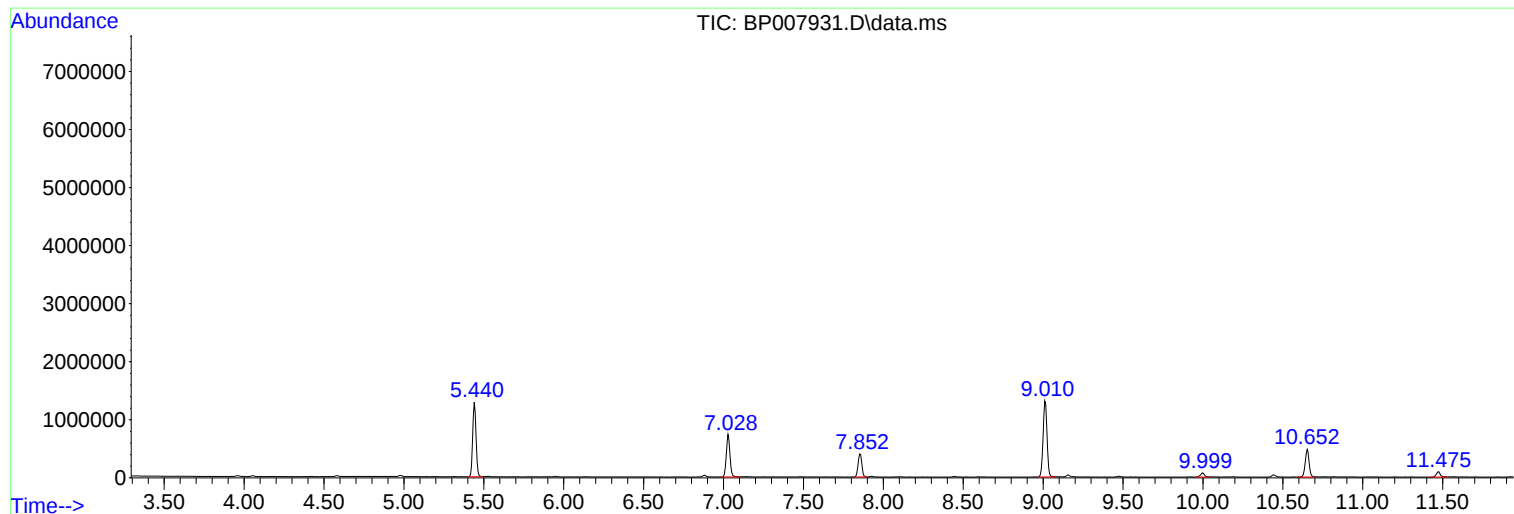
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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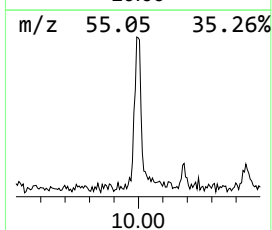
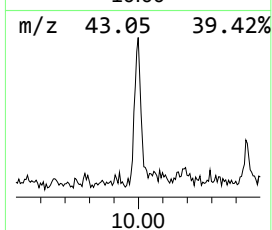
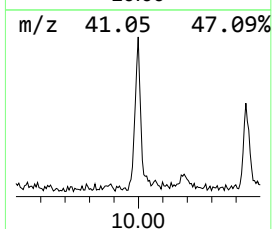
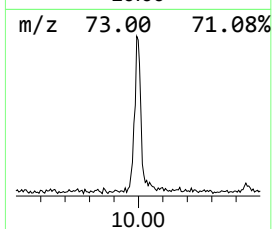
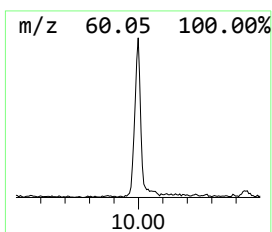
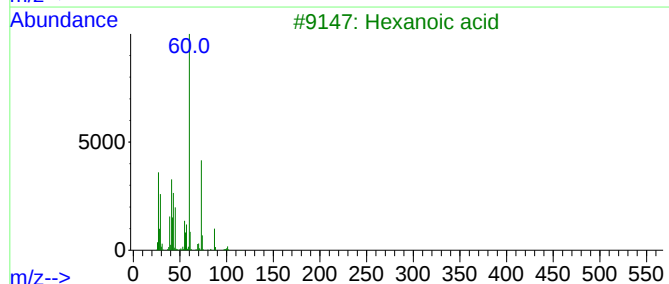
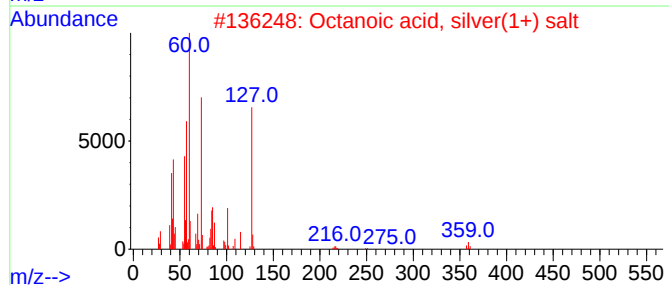
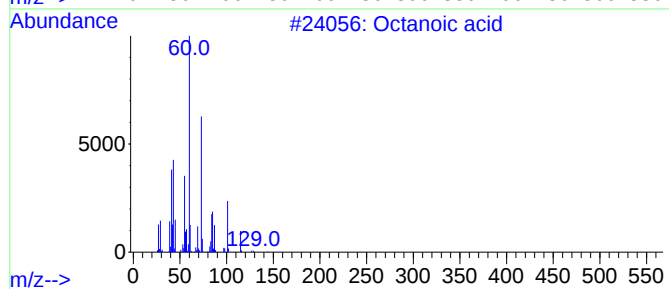
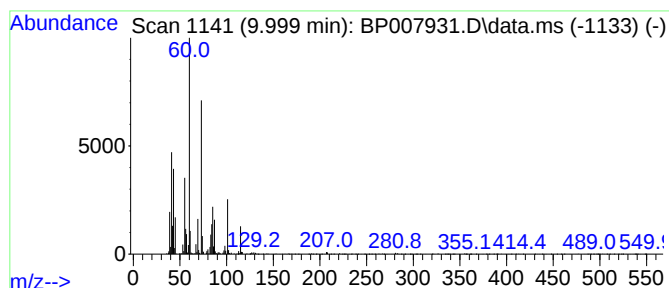
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Octanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.999	3.10 ng	124307	Naphthalene-d8	10.652

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid	144	C8H16O2	000124-07-2	90
2			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	72
3			Hexanoic acid	116	C6H12O2	000142-62-1	50
4			Pentanoic acid	102	C5H10O2	000109-52-4	47
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	47



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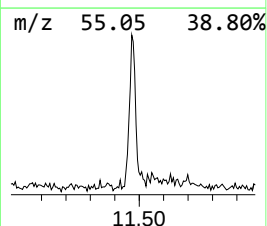
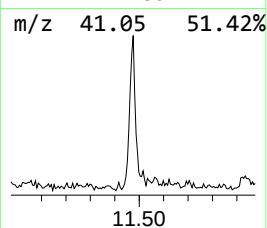
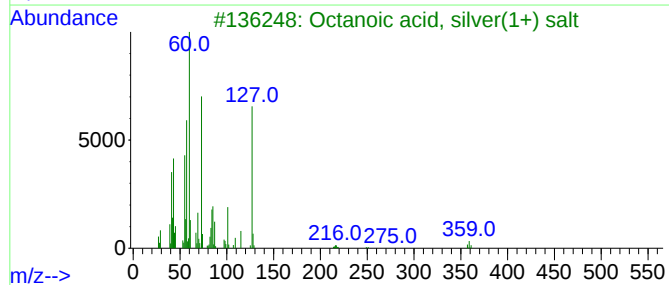
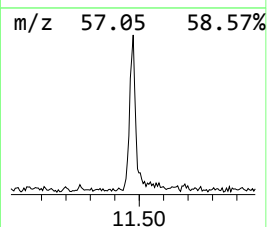
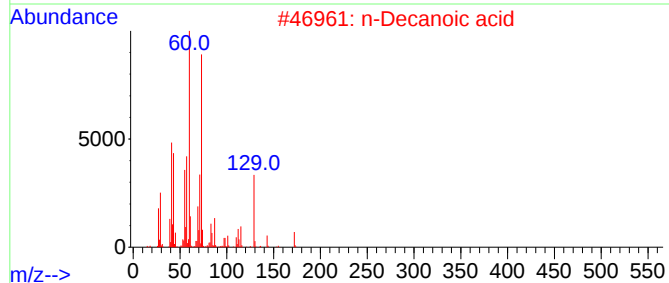
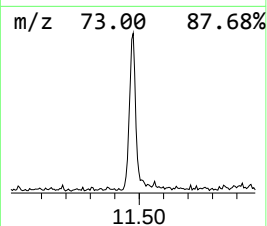
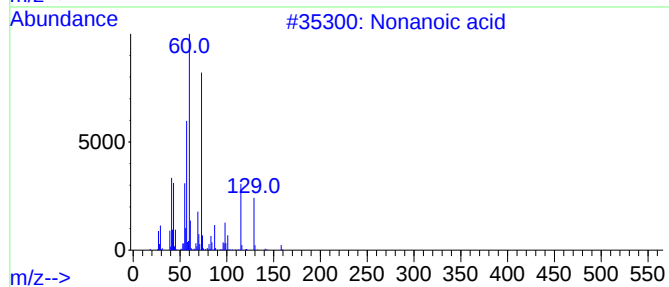
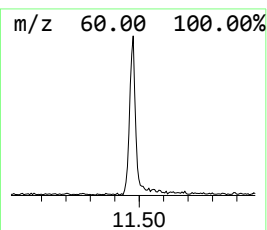
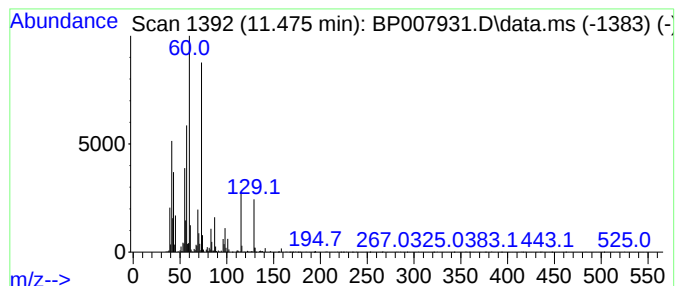
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Nonanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.475	4.24 ng	169971	Naphthalene-d8	10.652

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	95
2			n-Decanoic acid	172	C10H20O2	000334-48-5	72
3			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	50
4			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	43



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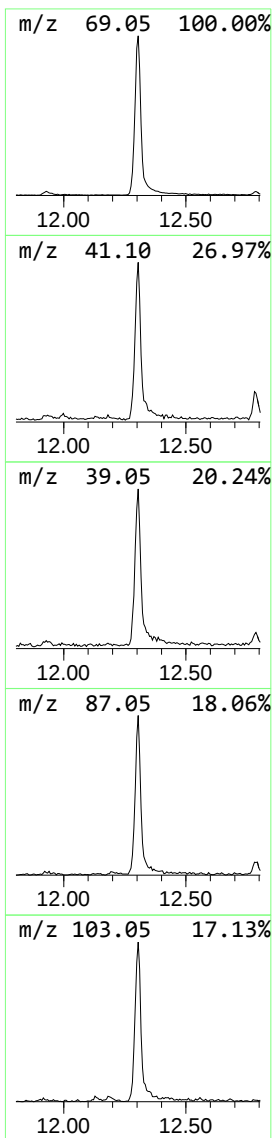
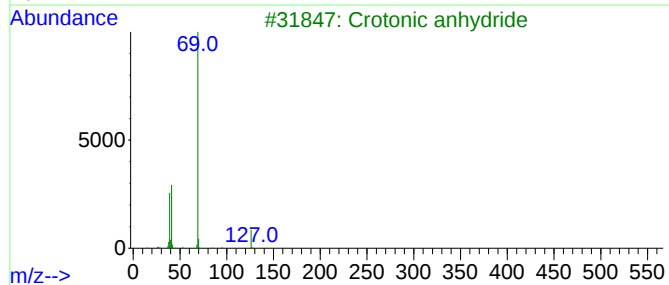
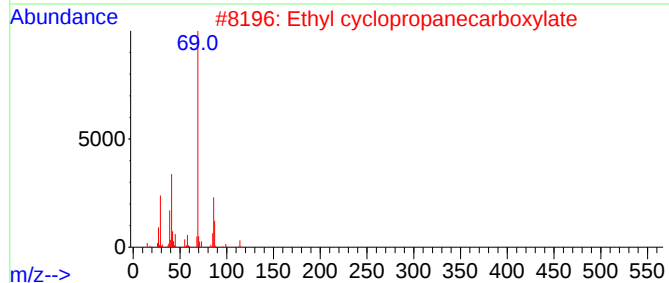
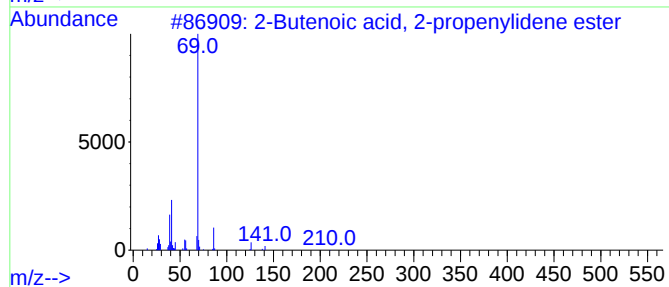
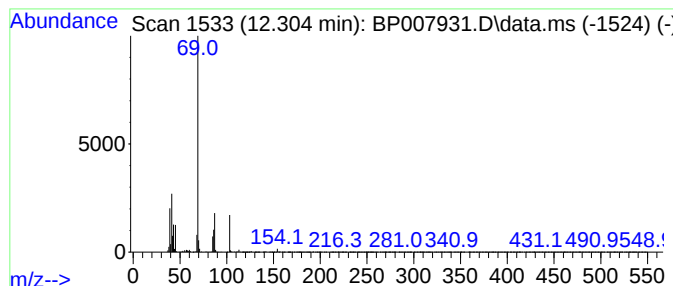
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Peak Number 3 unknown12.304 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	9.69 ng	388510	Naphthalene-d8	10.652

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
2			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
3			Crotonic anhydride	154	C8H10O3	000623-68-7	38
4			Isoamyl crotonate	156	C9H16O2	1010429-17-3	33
5			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	9



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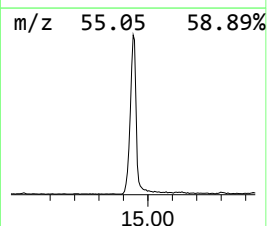
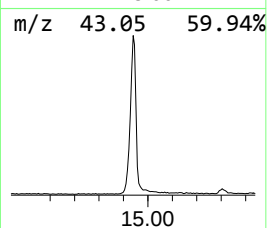
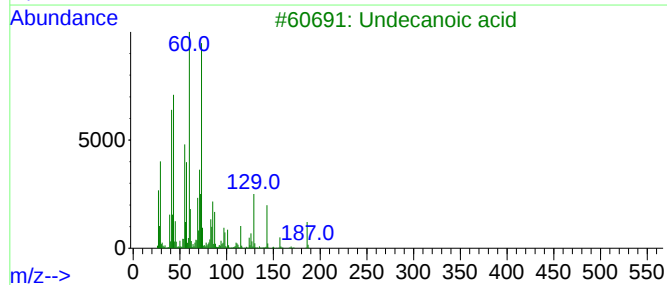
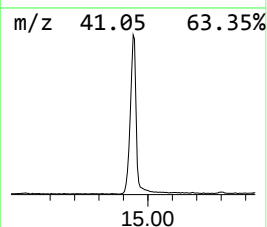
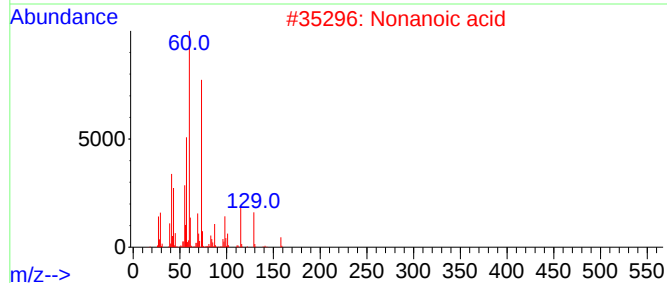
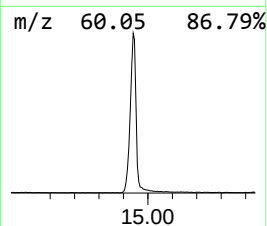
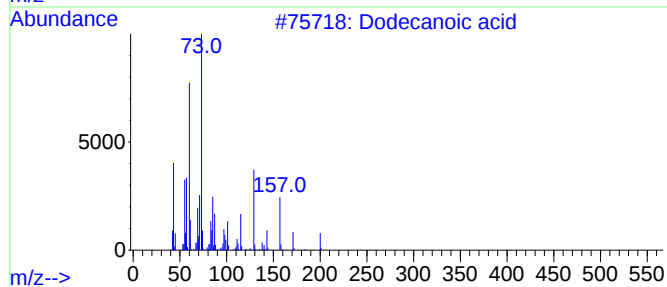
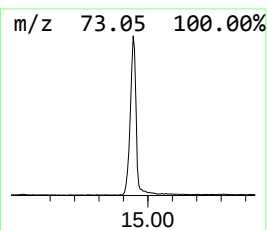
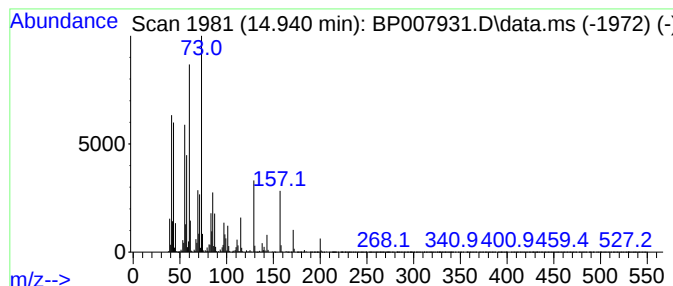
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.940	41.82 ng	2289120	Acenaphthene-d10	14.493

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	99
2			Nonanoic acid	158	C9H18O2	000112-05-0	62
3			Undecanoic acid	186	C11H22O2	000112-37-8	59
4			n-Decanoic acid	172	C10H20O2	000334-48-5	53
5			Octanoic acid	144	C8H16O2	000124-07-2	49



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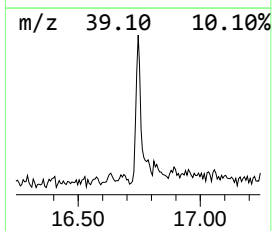
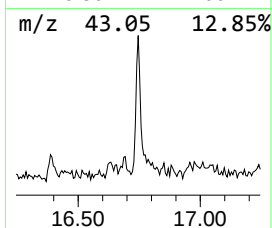
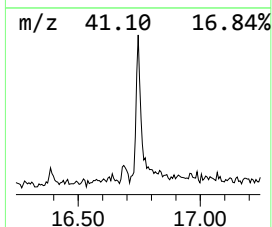
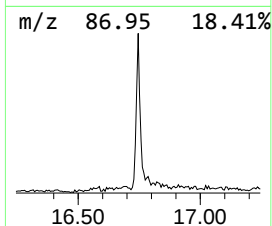
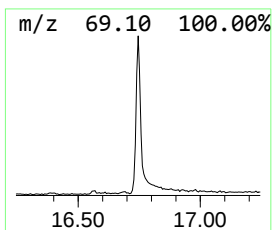
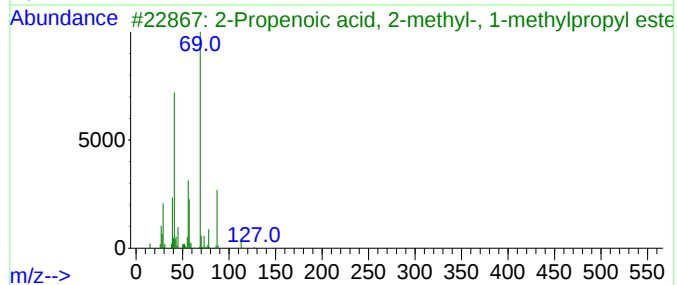
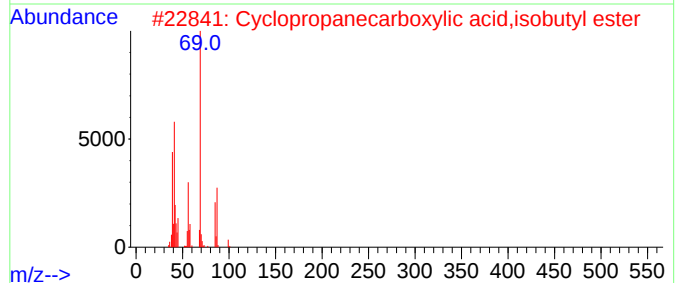
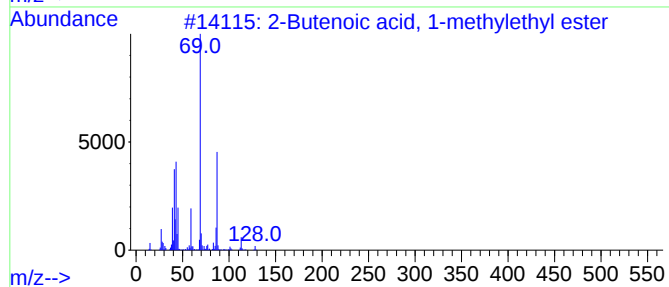
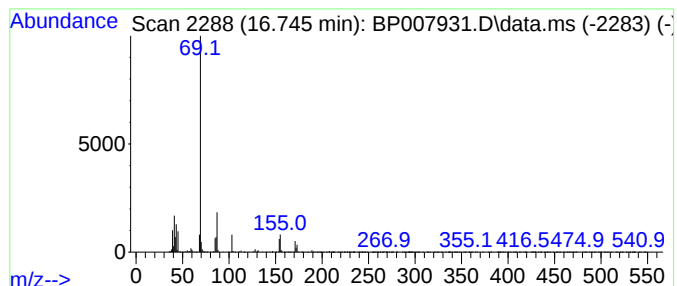
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Peak Number 5 2-Butenoic acid, 1-methylet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	2.75 ng	194975	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenoic acid, 1-methylethyl e...	128	C7H12O2	018060-77-0	59
2			Cyclopropanecarboxylic acid,isob...	142	C8H14O2	064969-79-5	42
3			2-Propenoic acid, 2-methyl-, 1-m...	142	C8H14O2	002998-18-7	36
4			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	36
5			3,3,7-Trimethyl-4-oxa-7-octen-1-ol	172	C10H20O2	069161-47-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Octanoic acid	9.999	3.1	ng	124307	2	10.652	801693	20.0
Nonanoic acid	11.475	4.2	ng	169971	2	10.652	801693	20.0
unknown12.304	12.304	9.7	ng	388510	2	10.652	801693	20.0
Dodecanoic acid	14.940	41.8	ng	2289120	3	14.493	1094730	20.0
2-Butenoic acid...	16.745	2.8	ng	194975	4	17.245	1418000	20.0