

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072121\
 Data File : BF124680.D
 Acq On : 22 Jul 2021 2:46
 Operator : JU/CG
 Sample : M3076-05
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210515-FIELD-BLANK-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_F\METHODS\8270-BF070721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124683.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	10	15	19	rBB	43071	52133	18.69%	4.068%
2	5.498	576	580	583	rBB	85246	73727	26.43%	5.752%
3	6.498	747	750	753	rBB	59491	44405	15.92%	3.465%
4	6.887	813	816	819	rBB	43315	30739	11.02%	2.398%
5	7.451	907	912	915	rBB	130885	123187	44.16%	9.611%
6	8.069	1014	1017	1020	rBB	14983	10586	3.79%	0.826%
7	8.169	1031	1034	1037	rBB	57899	43393	15.56%	3.386%
8	9.251	1213	1218	1221	rBB	301467	260545	93.40%	20.329%
9	9.928	1330	1333	1336	rBB	71795	51894	18.60%	4.049%
10	10.716	1463	1467	1470	rBB	176235	156611	56.14%	12.219%
11	11.410	1582	1585	1589	rBB	58913	51503	18.46%	4.018%
12	11.933	1671	1674	1678	rBB	22934	19886	7.13%	1.552%
13	12.721	1805	1808	1811	rBB	13783	9322	3.34%	0.727%
14	13.004	1851	1856	1859	rBV	298877	278956	100.00%	21.765%
15	13.892	2005	2007	2014	rBB	5866	6693	2.40%	0.522%
16	14.051	2031	2034	2037	rVB	46012	36140	12.96%	2.820%
17	15.527	2281	2285	2289	rBB	27118	31944	11.45%	2.492%

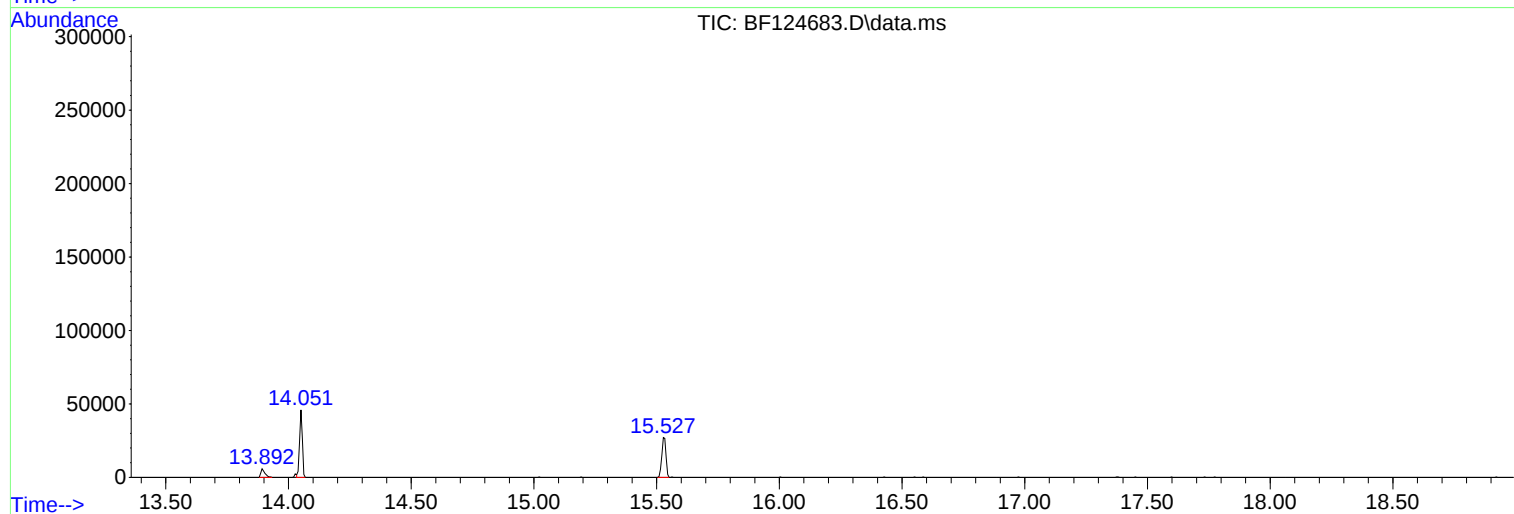
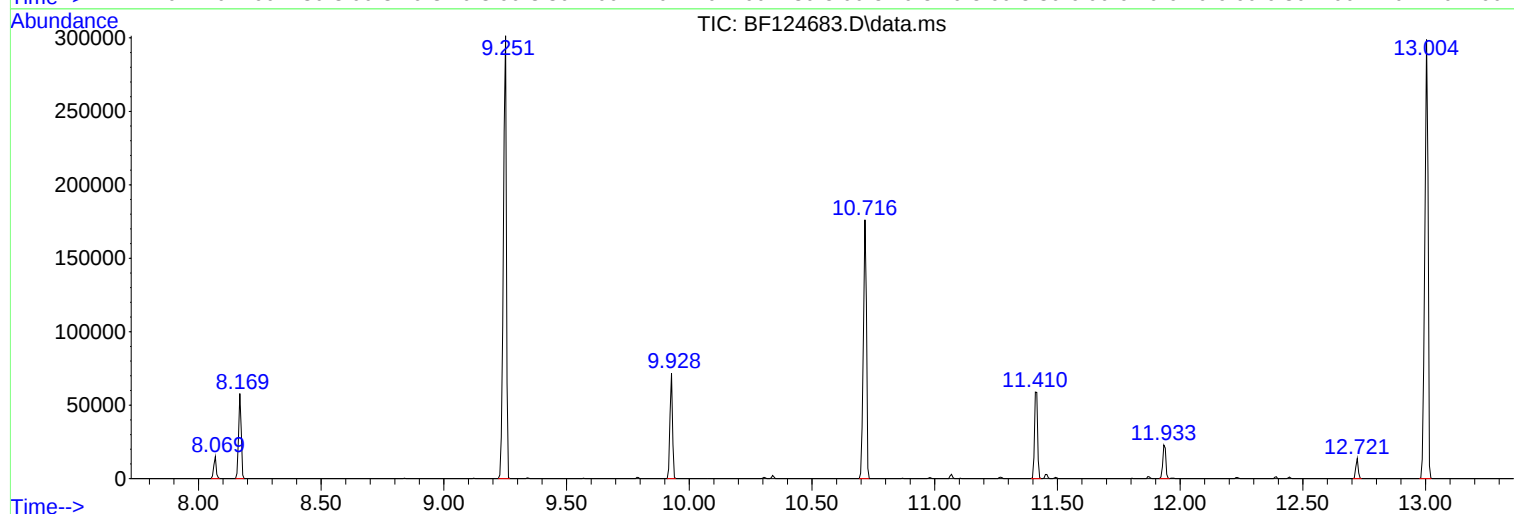
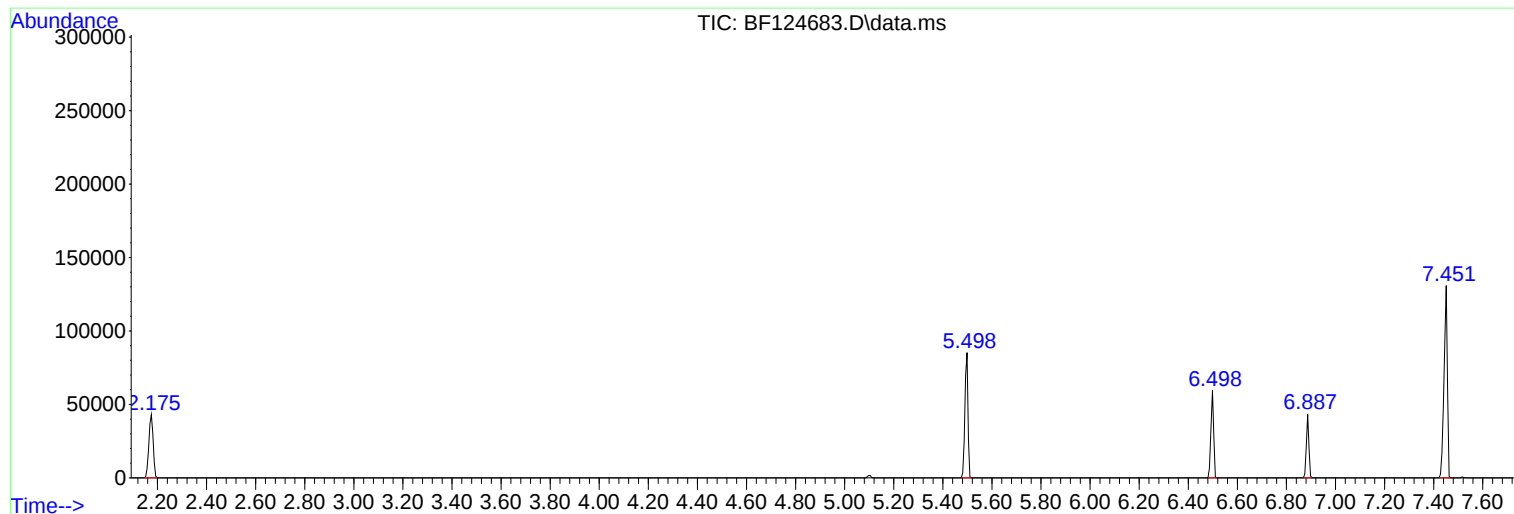
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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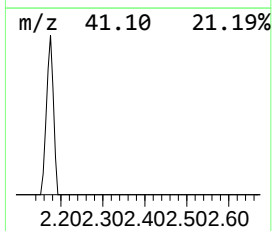
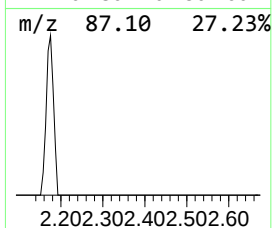
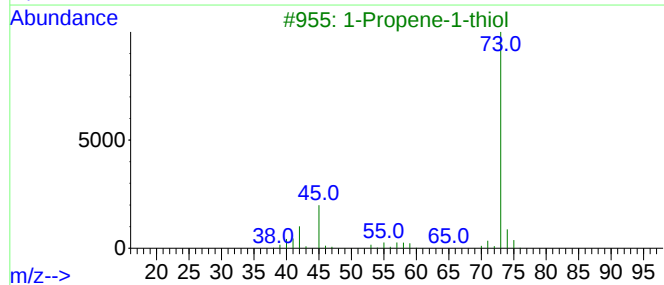
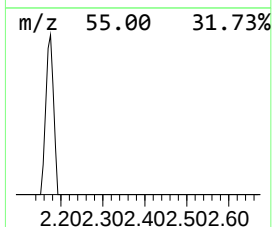
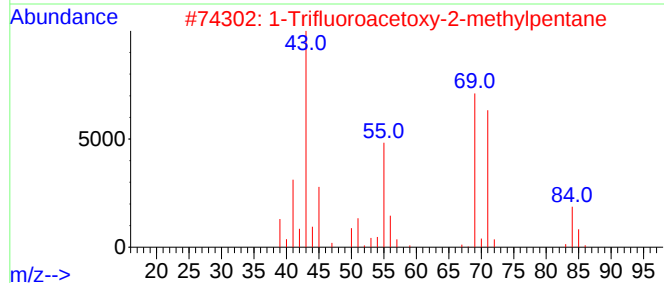
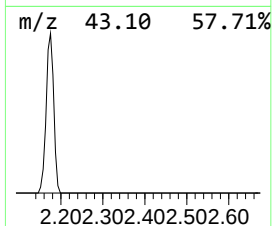
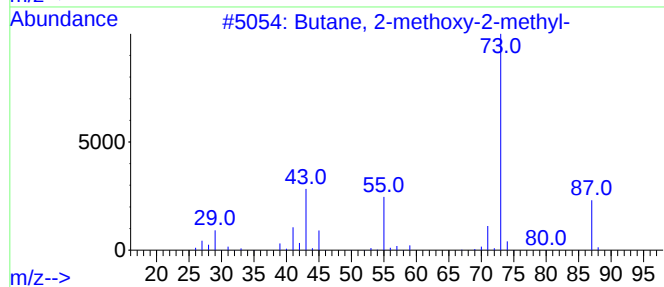
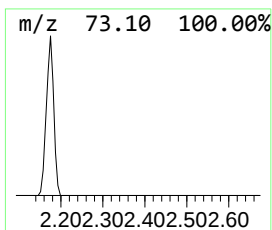
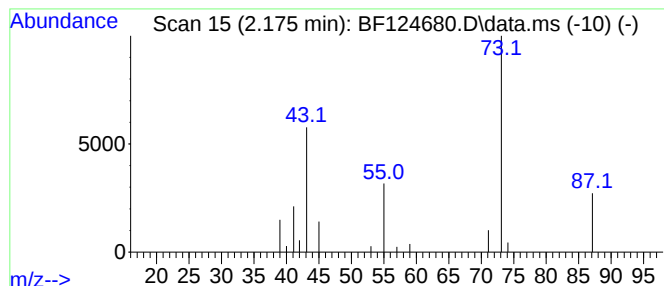
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.175	33.92 ng	52133	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	12
3			1-Propene-1-thiol	74	C3H6S	000925-89-3	9
4			Oxalic acid, allyl pentyl ester	200	C10H16O4	1000309-23-2	9
5			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9



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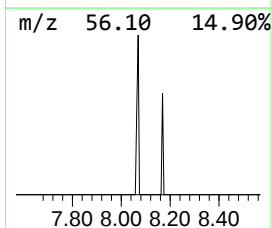
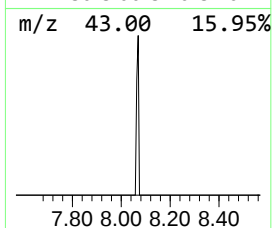
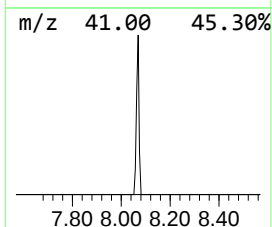
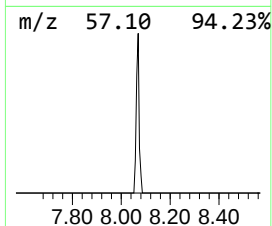
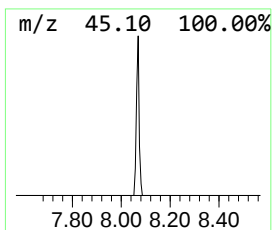
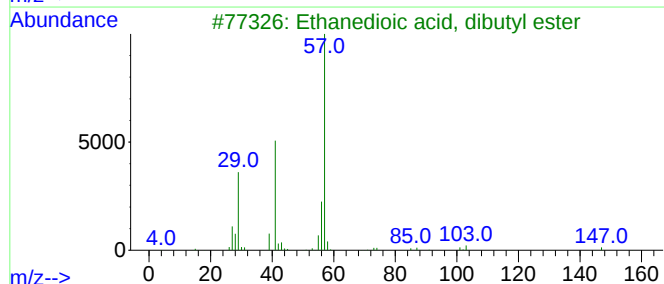
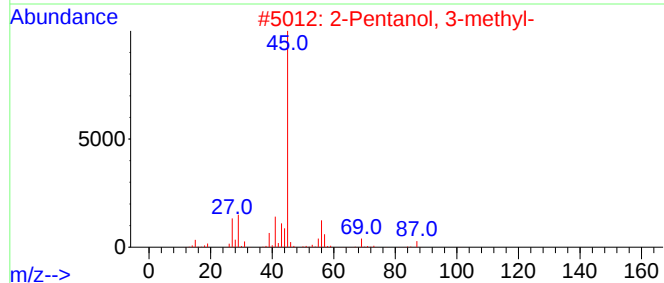
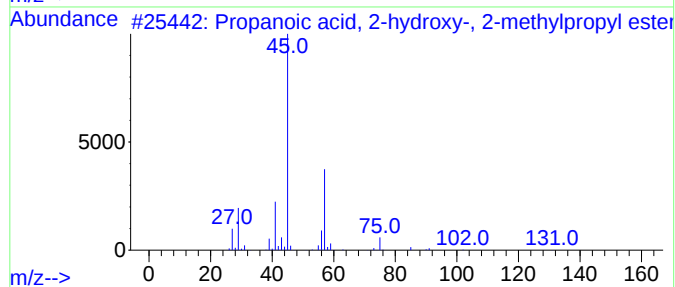
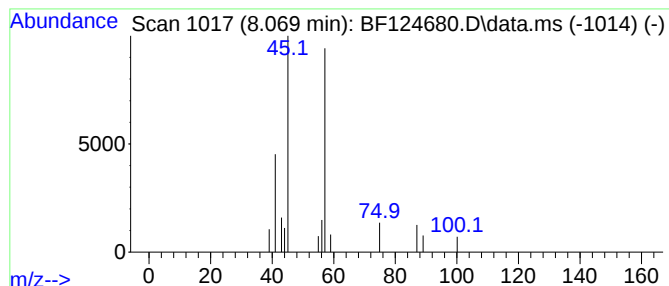
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown8.069 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	4.88 ng	10586	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	9
2			2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	9
3			Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	9
4			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	9
5			Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	9



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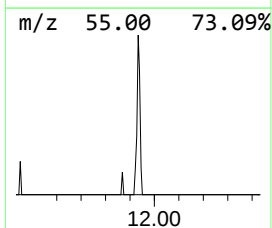
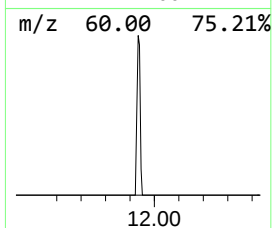
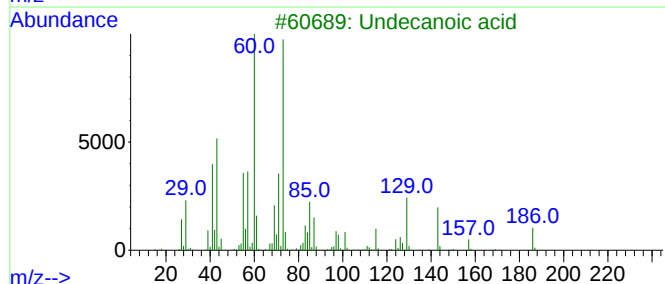
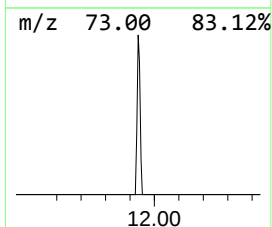
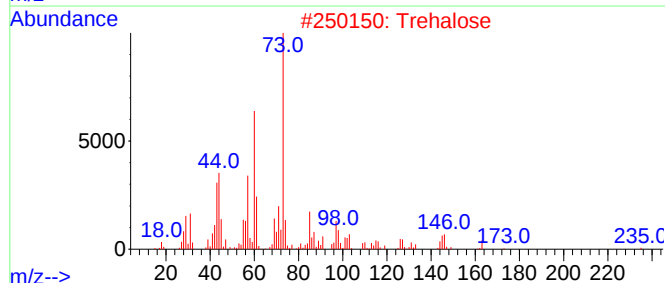
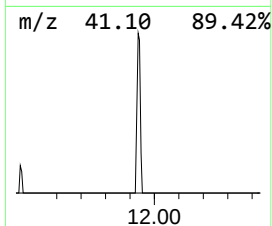
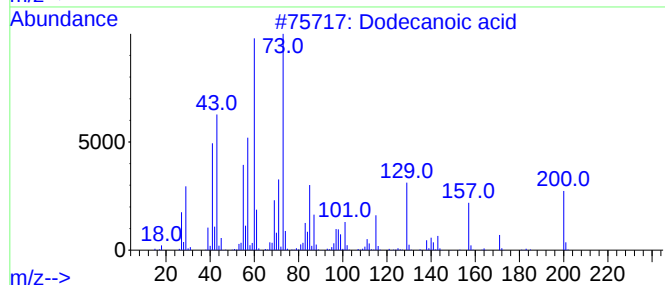
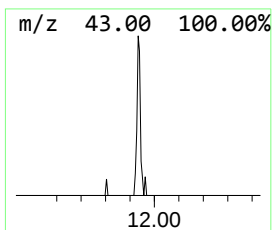
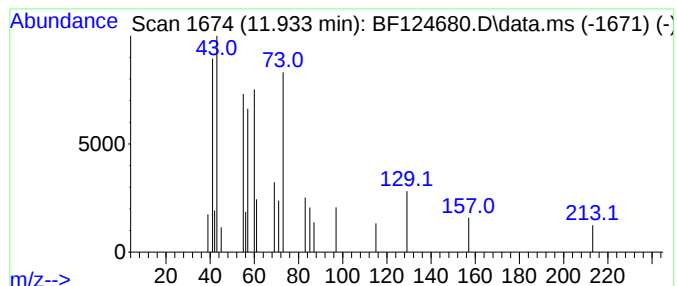
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	7.72 ng	19886	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	59
2			Trehalose	342	C12H22O11	000099-20-7	53
3			Undecanoic acid	186	C11H22O2	000112-37-8	50
4			n-Decanoic acid	172	C10H20O2	000334-48-5	47
5			Octanoic acid	144	C8H16O2	000124-07-2	47



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Misc :
ALS Vial : 20 Sample Multiplier: 1

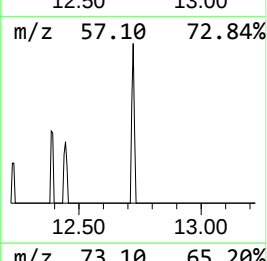
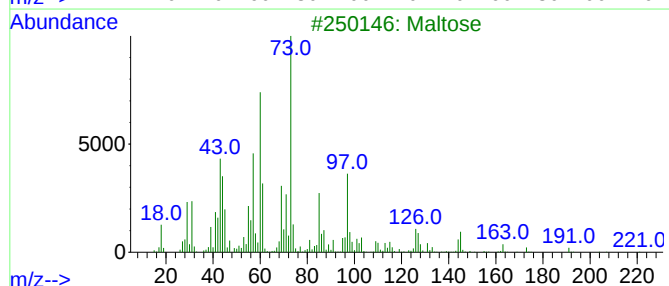
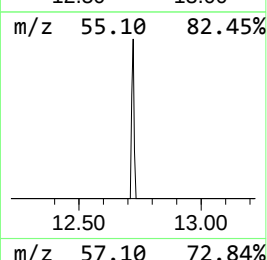
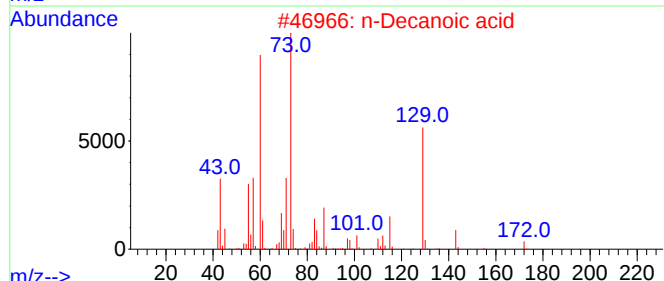
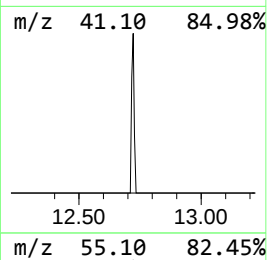
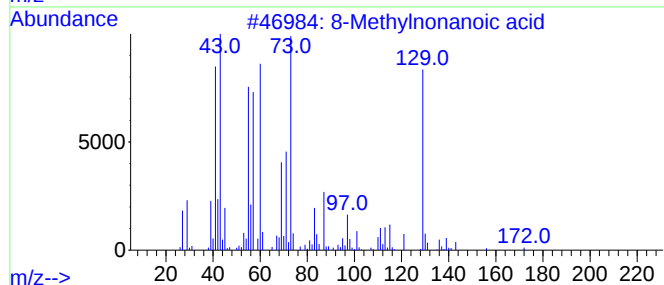
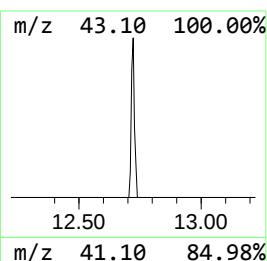
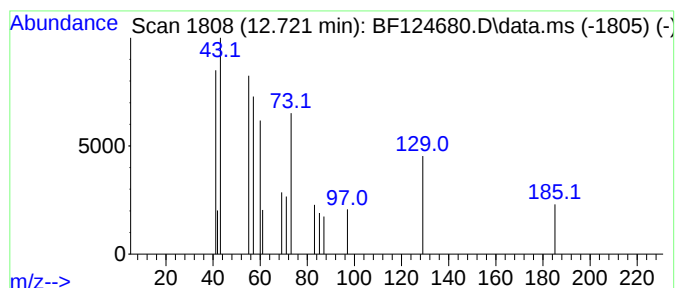
Instrument :
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Peak Number 4 8-Methylnonanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.722	3.62 ng	9322	Phenanthrene-d10		11.416	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	50
2	n-Decanoic acid		172	C10H20O2	000334-48-5	47
3	Maltose		342	C12H22O11	000069-79-4	43
4	l-Gala-1-ido-octose		240	C8H16O8	1000130-12-1	38
5	Propyl tetracosyl ether		396	C27H56O	1000406-28-3	35



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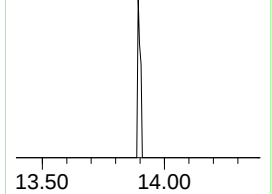
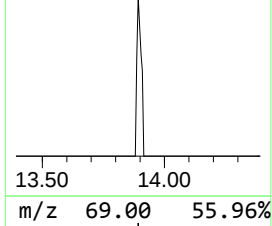
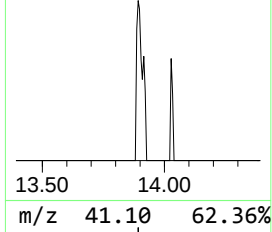
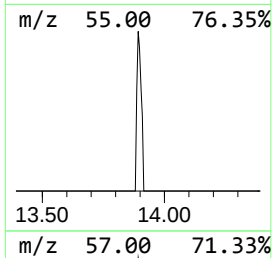
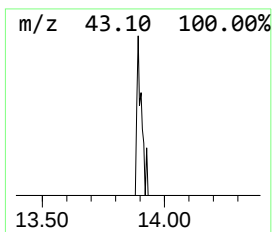
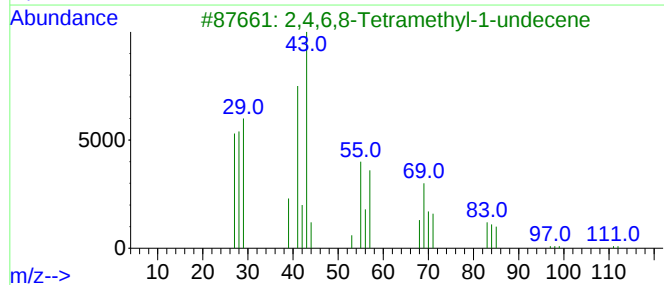
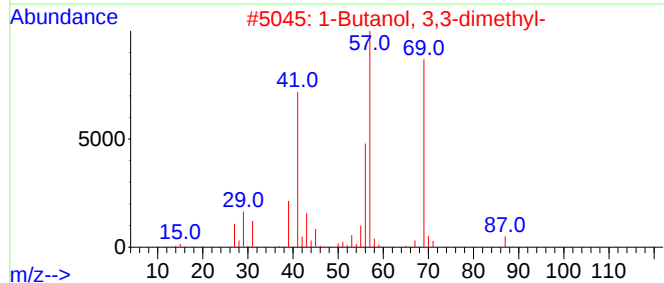
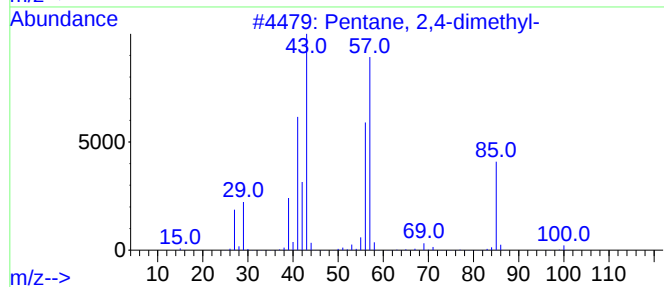
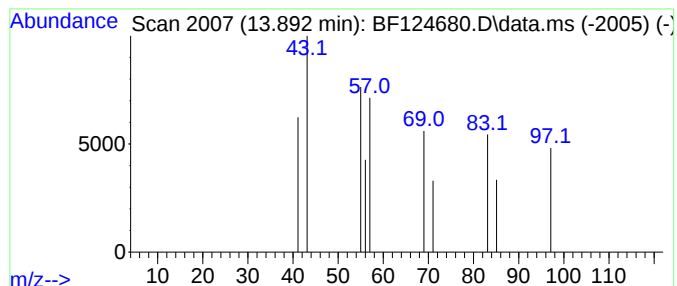
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown13.892 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.70 ng	6693	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	10
2			1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	9
3			2,4,6,8-Tetramethyl-1-undecene	210	C15H30	059920-26-2	9
4			Pentane, 2-chloro-2-methyl-	120	C6H13Cl	004325-48-8	8
5			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	33.9	ng	52133	1	6.887	30739	20.0
unknown8.069	8.069	4.9	ng	10586	2	8.169	43393	20.0
Dodecanoic acid	11.933	7.7	ng	19886	4	11.416	51503	20.0
8-Methylnonanoi...	12.722	3.6	ng	9322	4	11.416	51503	20.0
unknown13.892	13.892	3.7	ng	6693	5	14.051	36140	20.0