

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020224\
 Data File : BF137256.D
 Acq On : 02 Feb 2024 15:47
 Operator : CG\JU
 Sample : P1337-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3

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-BF013024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137256.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	14	rVB	220090	291804	11.26%	1.936%
2	5.051	500	504	513	rBV	48890	72733	2.81%	0.483%
3	5.434	564	569	572	rBV	2174197	2192221	84.56%	14.547%
4	6.093	677	681	688	rBV	38530	48942	1.89%	0.325%
5	6.428	733	738	741	rBV	1944423	2201127	84.90%	14.606%
6	6.792	796	800	809	rBV	328342	314538	12.13%	2.087%
7	7.351	890	895	911	rBV	1301207	1452853	56.04%	9.641%
8	8.069	1013	1017	1026	rBV	439337	418386	16.14%	2.776%
9	9.145	1195	1200	1212	rBV	2666652	2592622	100.00%	17.204%
10	9.822	1311	1315	1323	rBV	591295	474968	18.32%	3.152%
11	10.616	1445	1450	1453	rBV	1722606	1549281	59.76%	10.280%
12	11.310	1565	1568	1577	rBV	450885	424133	16.36%	2.814%
13	11.857	1657	1661	1672	rBV	79116	129039	4.98%	0.856%
14	12.110	1700	1704	1707	rBV	64878	51962	2.00%	0.345%
15	12.916	1836	1841	1844	rBV	2394426	2235302	86.22%	14.833%
16	13.963	2015	2019	2030	rBV	381564	370338	14.28%	2.457%
17	15.439	2266	2270	2278	rBV	179882	249855	9.64%	1.658%

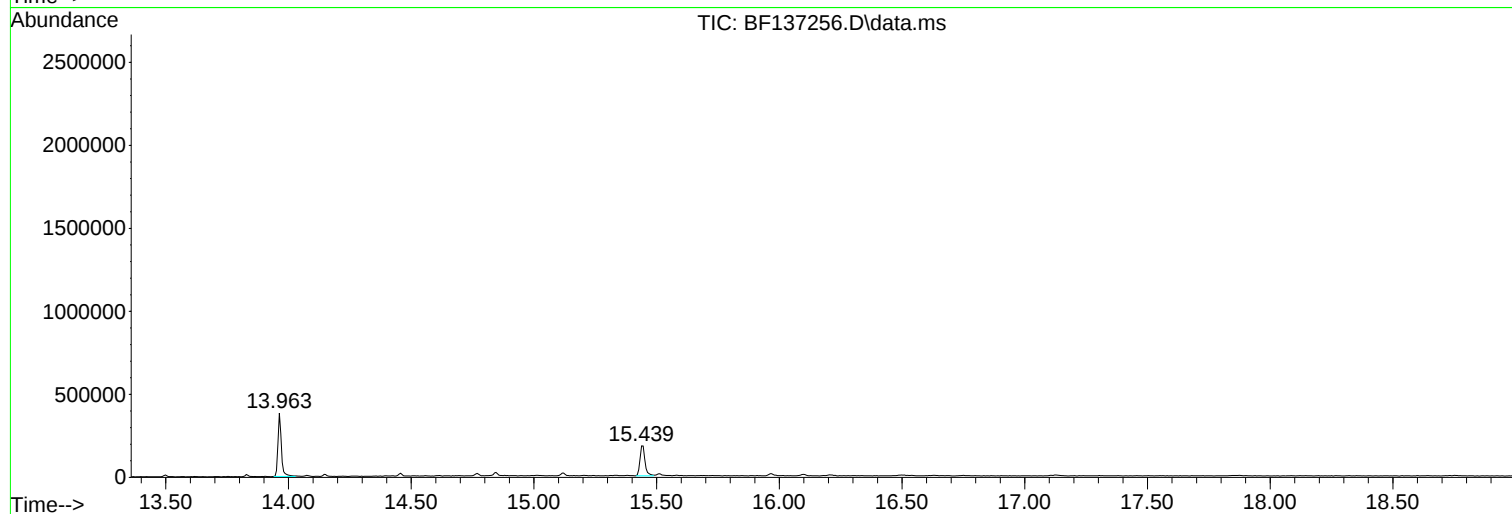
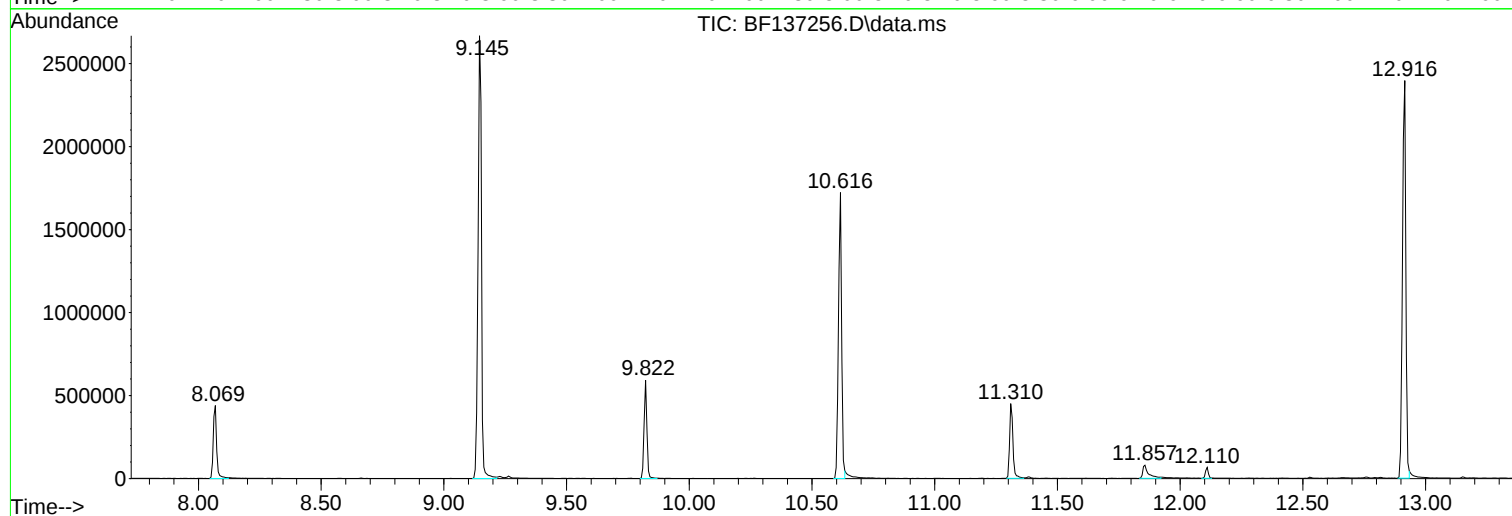
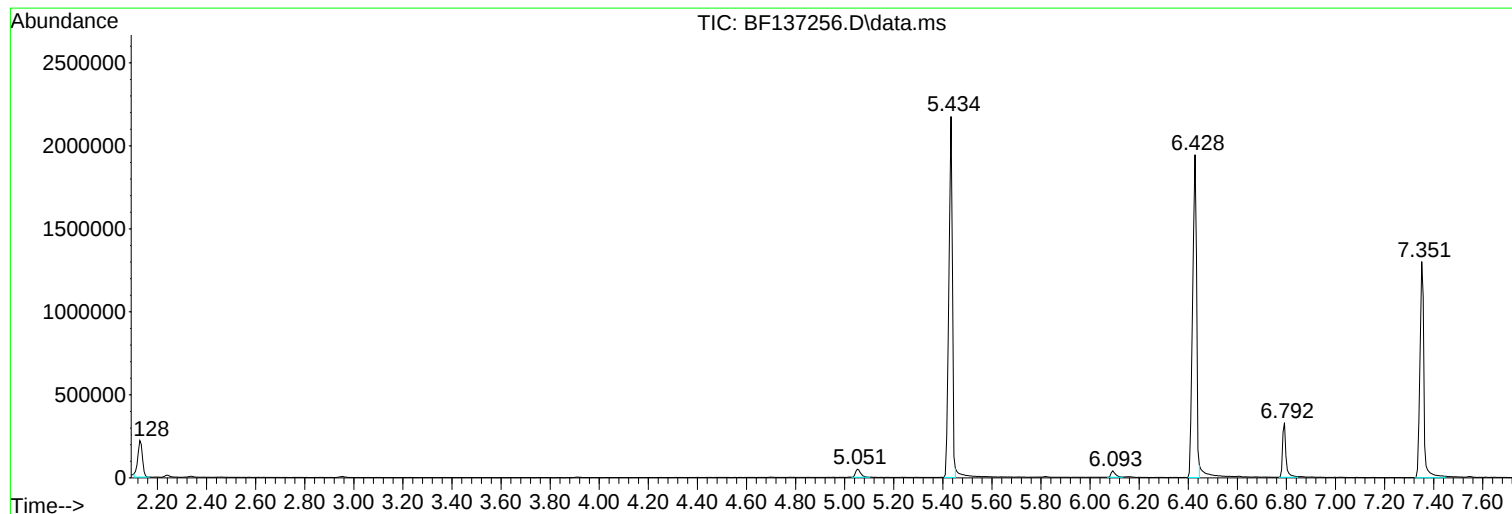
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
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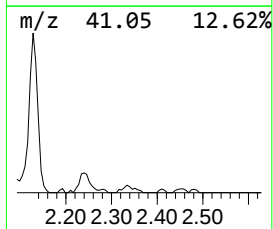
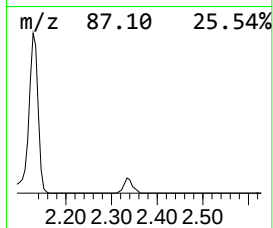
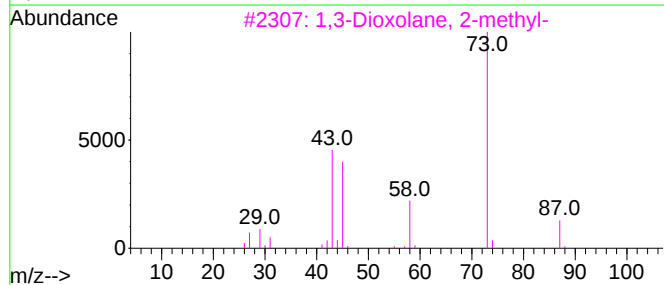
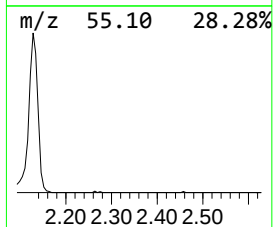
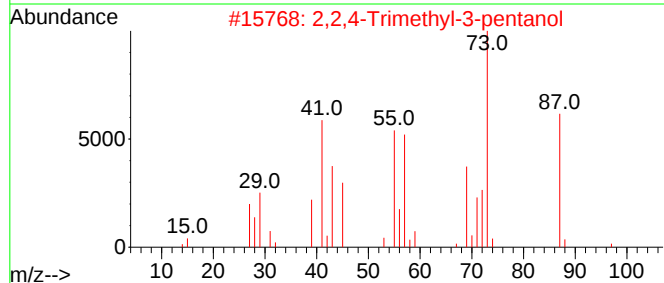
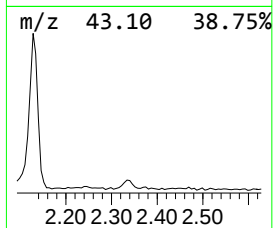
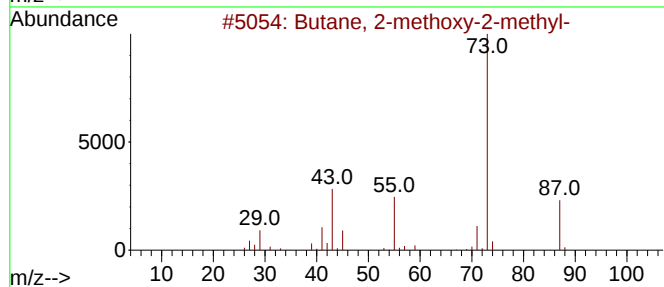
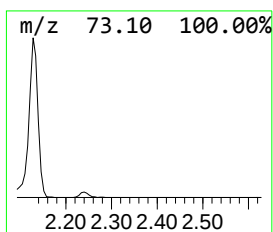
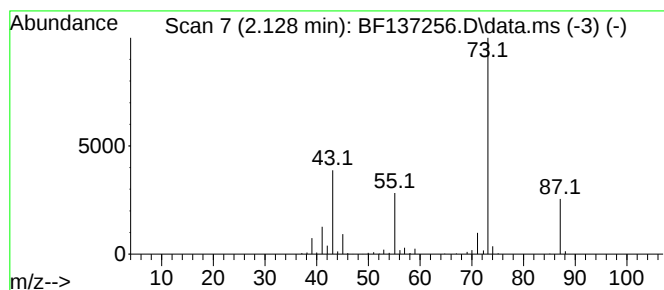
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.128	18.55 ng	291804	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23



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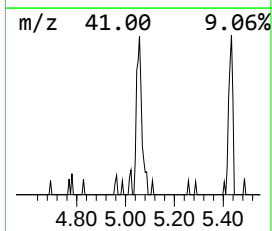
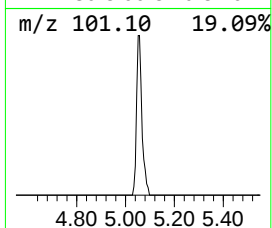
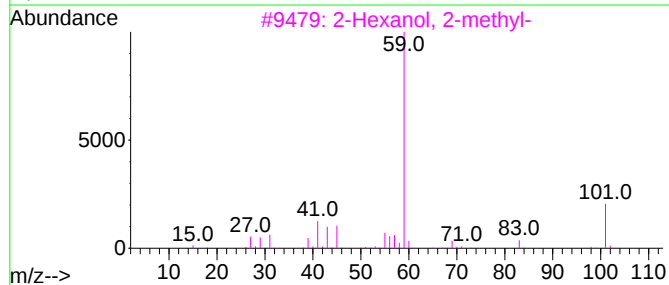
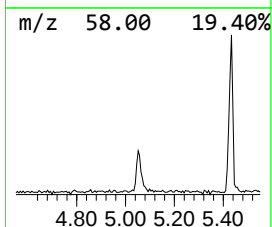
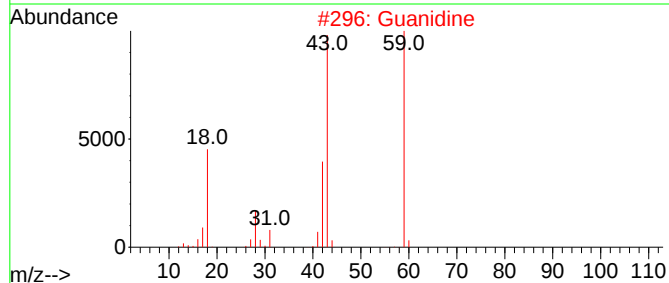
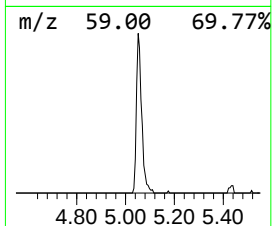
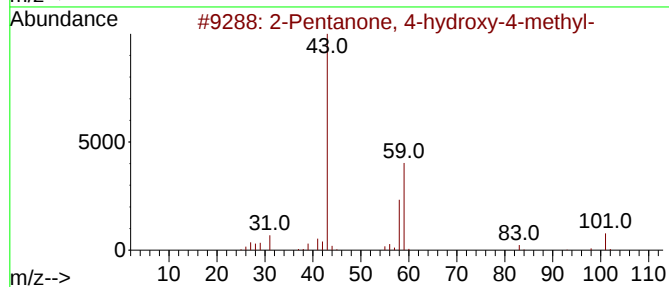
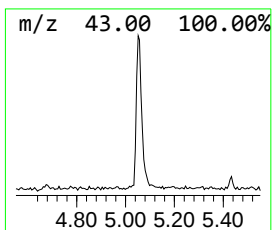
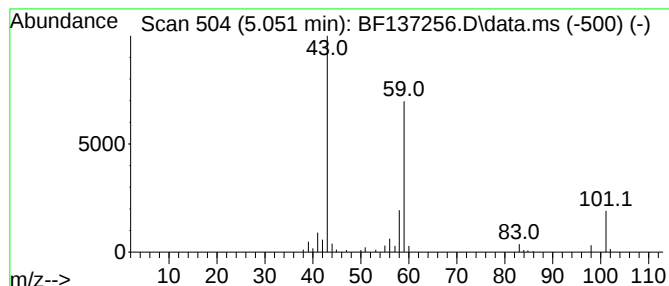
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	4.62 ng	72733	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42		
2	Guanidine	59	CH5N3	000113-00-8	38		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
4	3-Octanol	130	C8H18O	000589-98-0	28		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	17		



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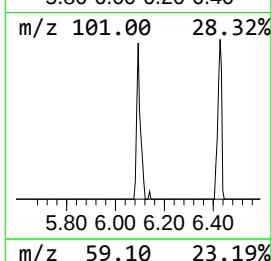
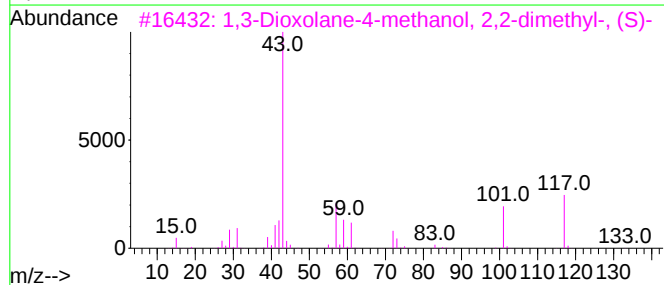
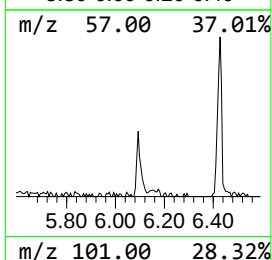
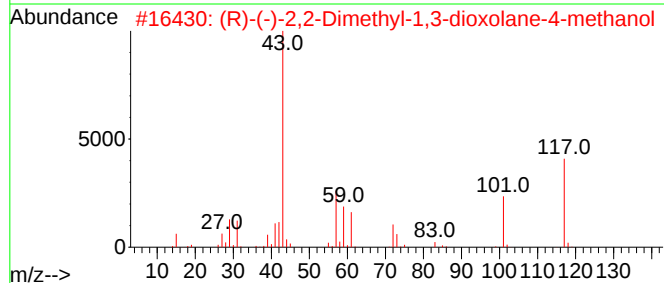
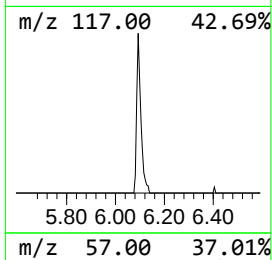
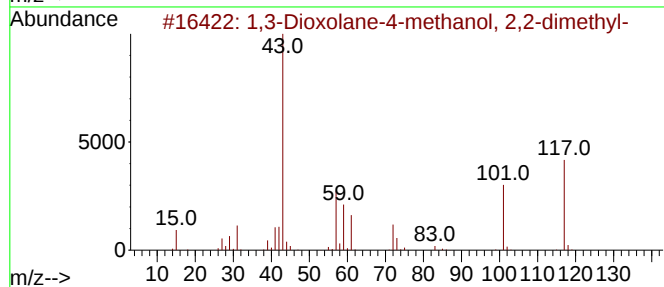
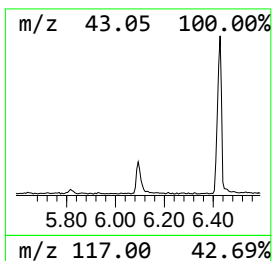
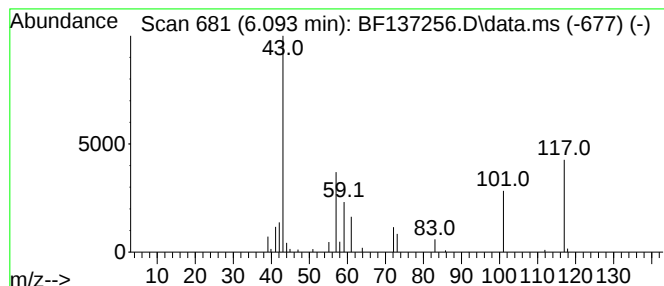
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,3-Dioxolane-4-methanol, 2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.093	3.11 ng	48942	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	000100-79-8	83
2			(R)-(-)-2,2-Dimethyl-1,3-dioxola...	132	C6H12O3	014347-78-5	83
3			1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	022323-82-6	59
4			n-Propyl acetate	102	C5H10O2	000109-60-4	12
5			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12



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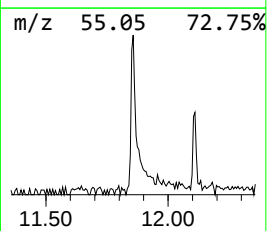
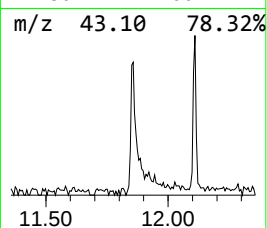
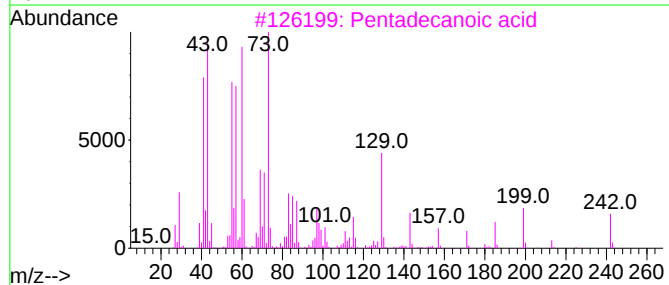
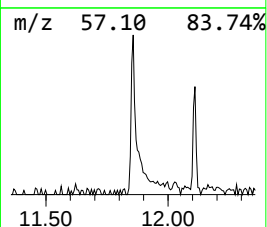
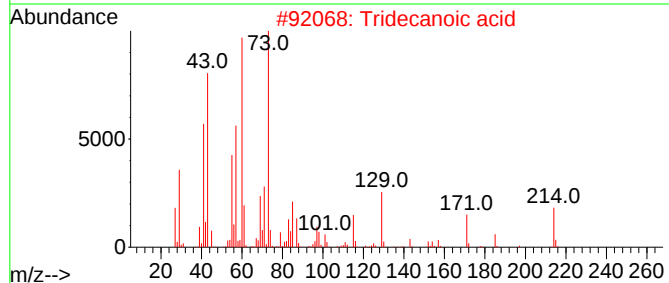
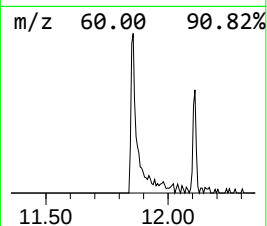
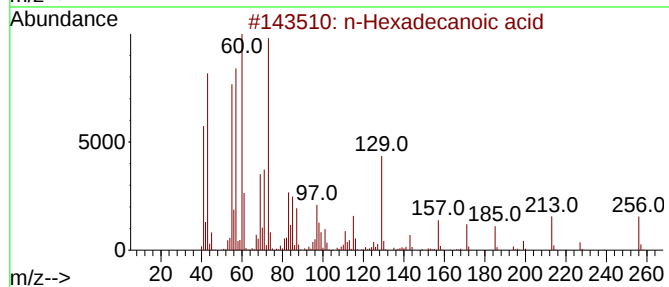
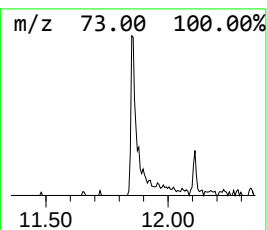
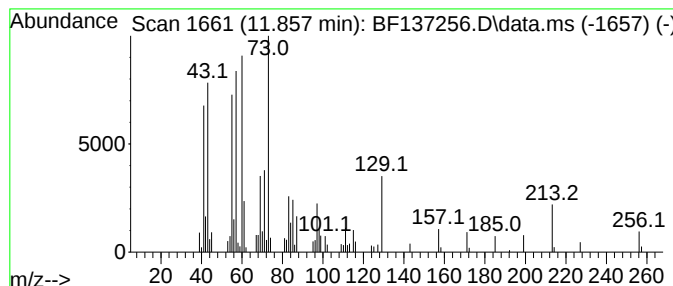
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	6.08 ng	129039	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Nonanoic acid	158	C9H18O2	000112-05-0	46



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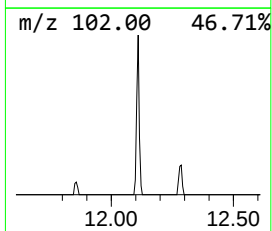
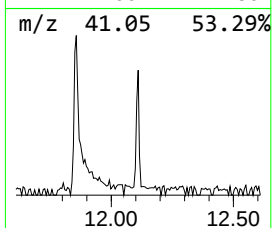
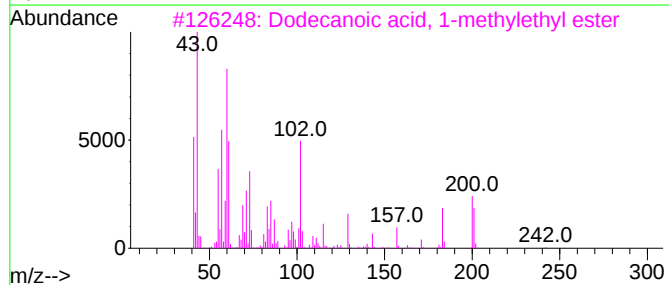
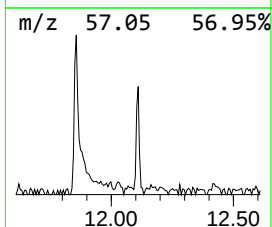
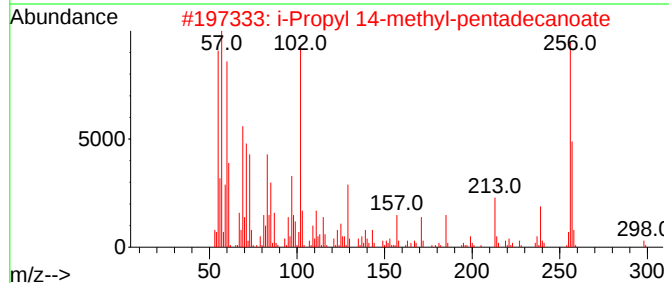
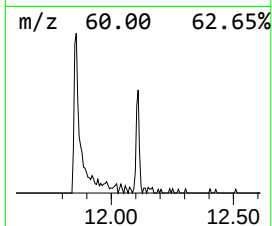
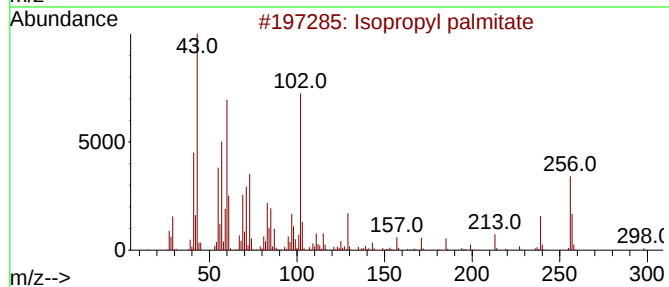
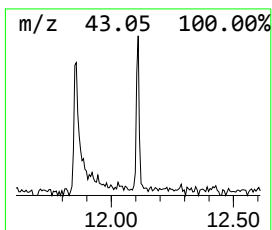
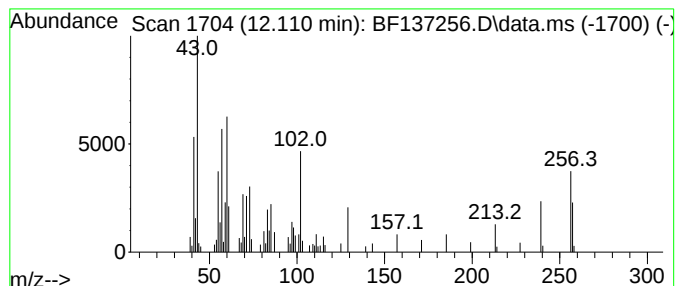
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl palmitate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.110	2.45 ng	51962	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	72
2			i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	49
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	46
4			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	43
5			8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	43



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.128	18.6	ng	291804	1	6.792	314538	20.0
2-Pentanone, 4-...	5.051	4.6	ng	72733	1	6.792	314538	20.0
1,3-Dioxolane-4...	6.093	3.1	ng	48942	1	6.792	314538	20.0
n-Hexadecanoic ...	11.857	6.1	ng	129039	4	11.310	424133	20.0
Isopropyl palmi...	12.110	2.5	ng	51962	4	11.310	424133	20.0