

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081024\
 Data File : BF138912.D
 Acq On : 10 Aug 2024 16:20
 Operator : RC/JU
 Sample : P3466-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 932-K1-WP0-0.25-080224

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-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138912.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	7	20	rVB	1758419	2681464	100.00%	24.372%
2	5.063	500	505	516	rVB	59801	93007	3.47%	0.845%
3	5.469	569	574	592	rBV	619553	867366	32.35%	7.884%
4	6.481	741	746	759	rBV	473609	621799	23.19%	5.652%
5	6.840	802	807	812	rBV	188988	232012	8.65%	2.109%
6	7.404	897	903	908	rBV	741249	982550	36.64%	8.931%
7	8.116	1019	1024	1038	rBV	236070	312451	11.65%	2.840%
8	8.440	1070	1079	1089	rBV	17022	34575	1.29%	0.314%
9	9.192	1201	1207	1212	rBV	1361575	1718654	64.09%	15.621%
10	9.869	1317	1322	1334	rBV	274411	348971	13.01%	3.172%
11	10.251	1382	1387	1393	rBV	21131	27621	1.03%	0.251%
12	10.663	1452	1457	1468	rBV	745995	986809	36.80%	8.969%
13	11.357	1570	1575	1585	rBV	269559	340440	12.70%	3.094%
14	11.880	1659	1664	1674	rBV4	16520	31601	1.18%	0.287%
15	12.751	1808	1812	1817	rBV	30285	36323	1.35%	0.330%
16	12.939	1839	1844	1849	rBV	1002801	1273398	47.49%	11.574%
17	13.833	1991	1996	2008	rBV9	9837	29804	1.11%	0.271%
18	13.998	2019	2024	2031	rVB	141493	177703	6.63%	1.615%
19	15.463	2267	2273	2281	rBV	134673	205572	7.67%	1.868%

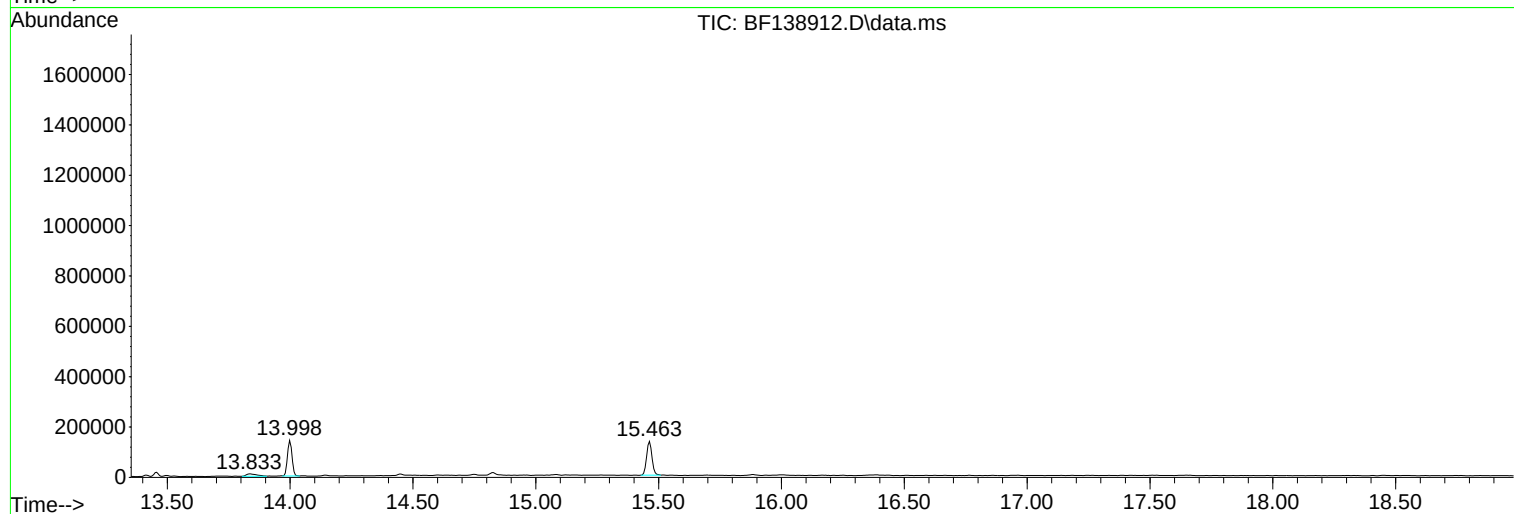
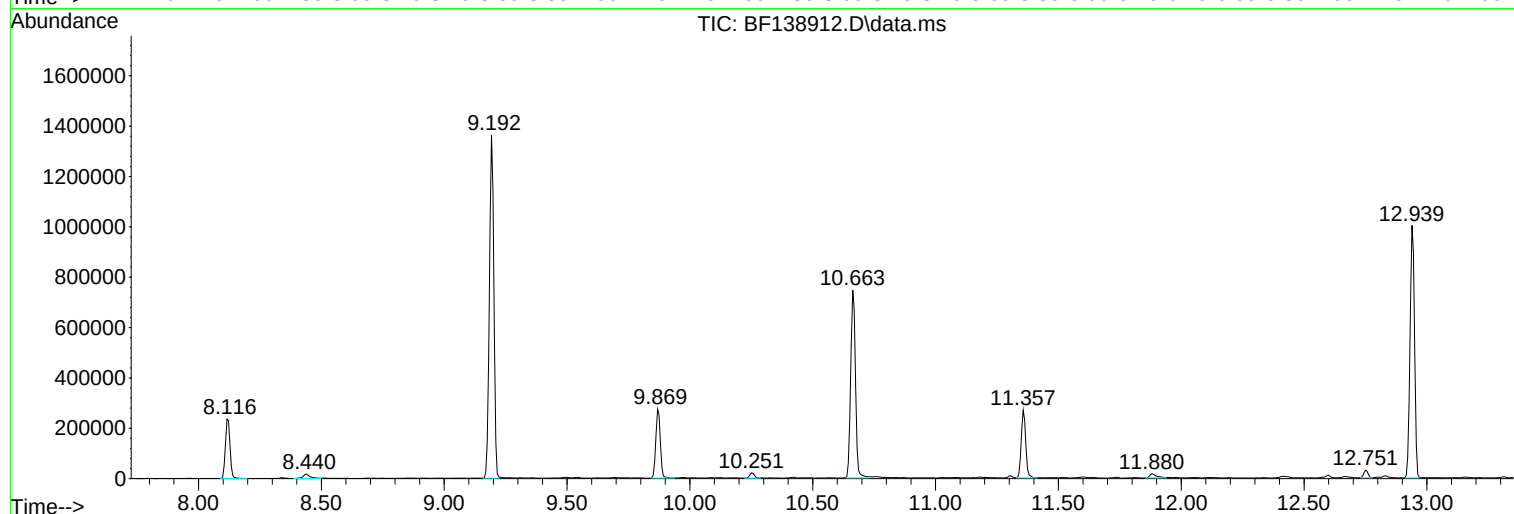
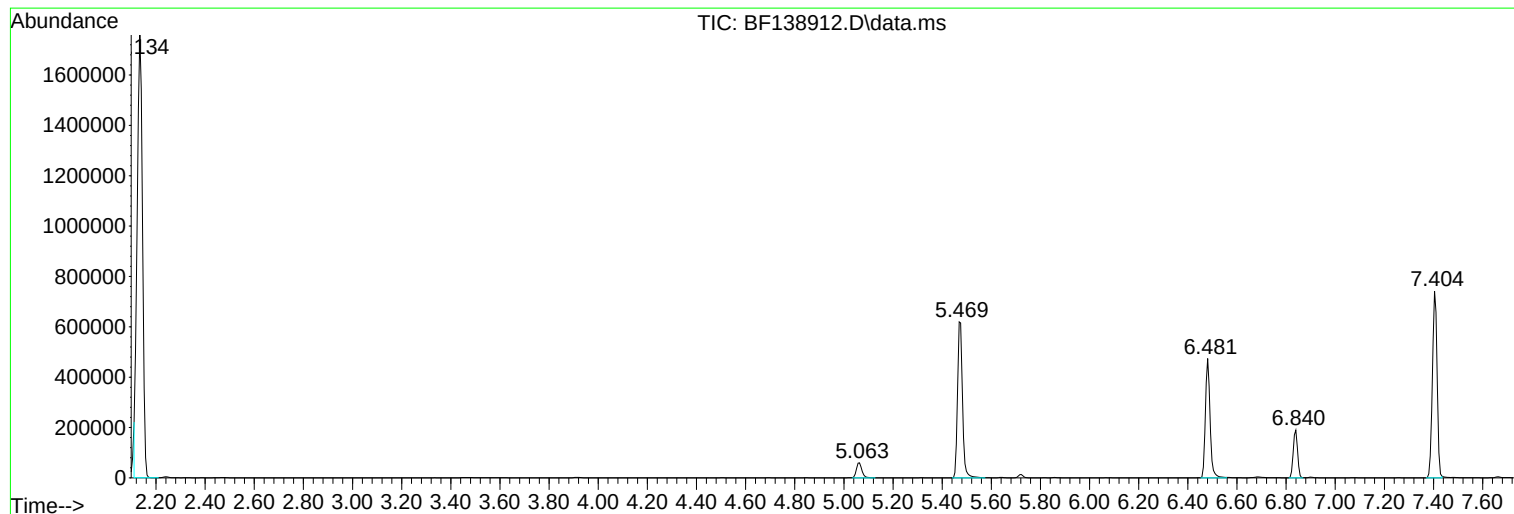
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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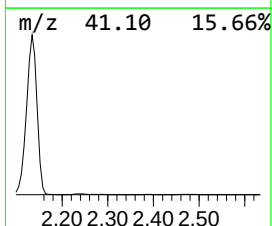
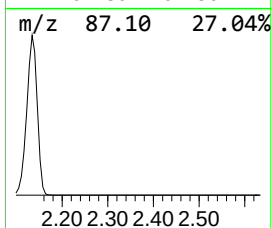
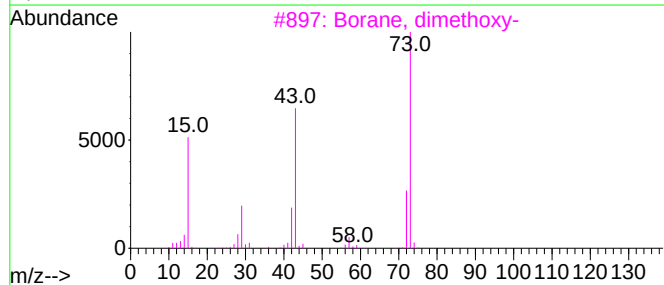
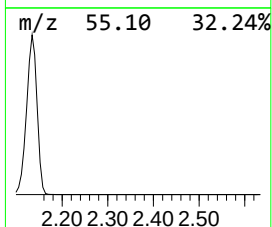
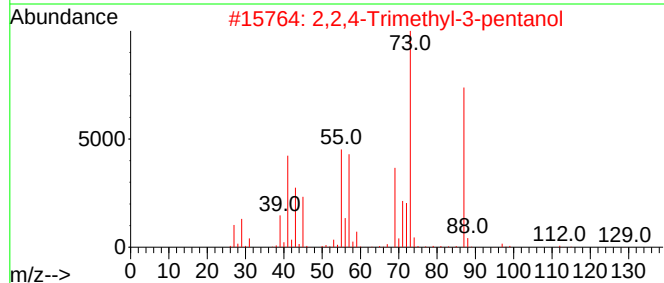
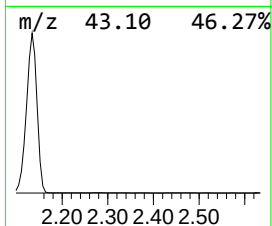
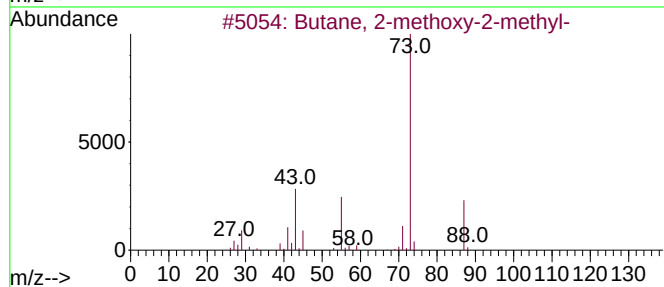
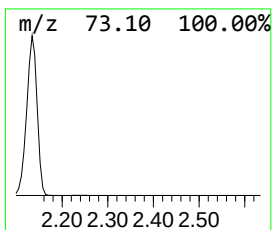
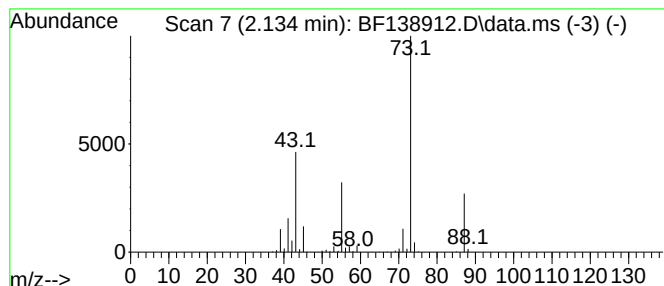
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	231.15 ng	2681460	1,4-Dichlorobenzene-d4	6.840

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	39
3			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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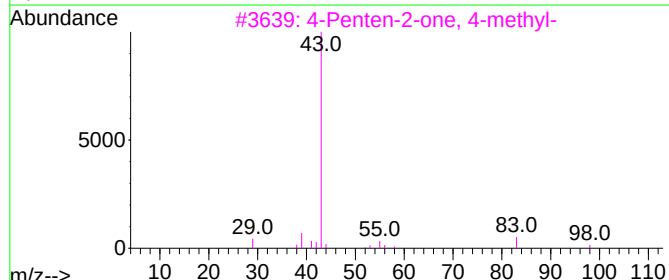
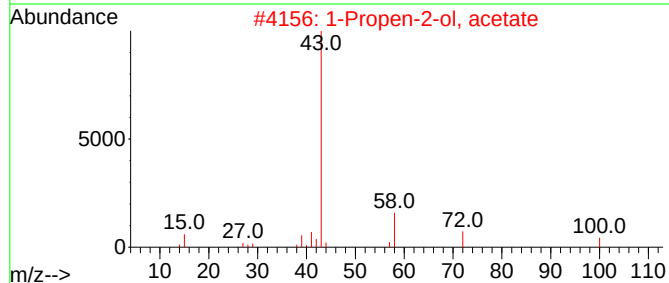
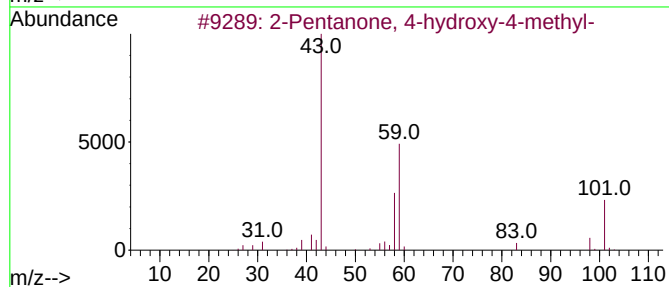
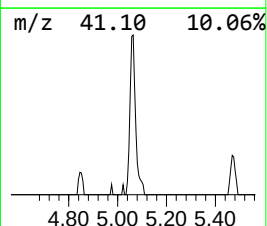
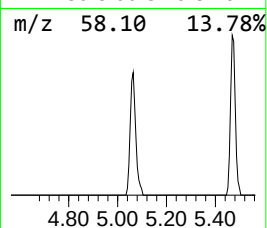
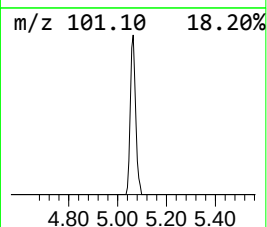
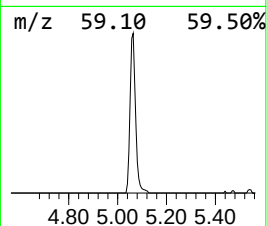
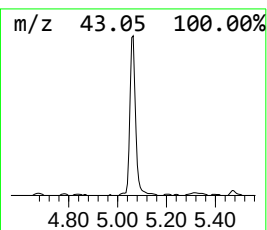
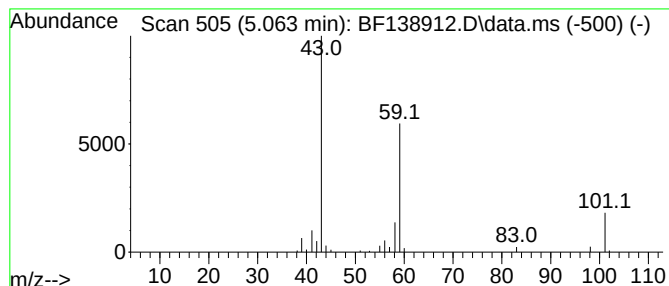
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	8.02 ng	93007	1,4-Dichlorobenzene-d4	6.840

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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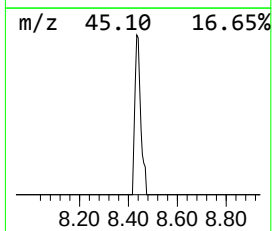
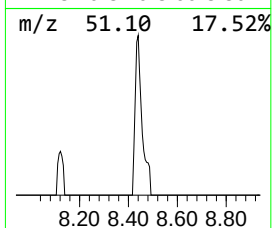
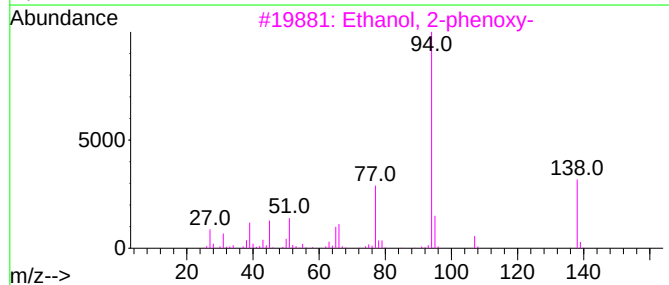
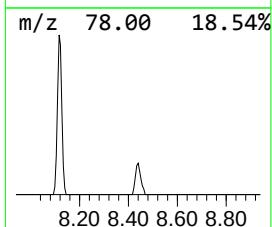
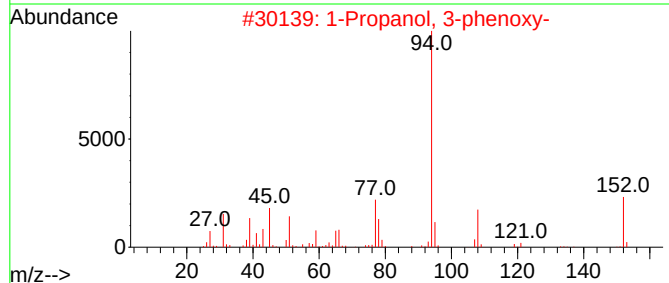
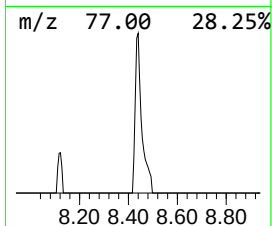
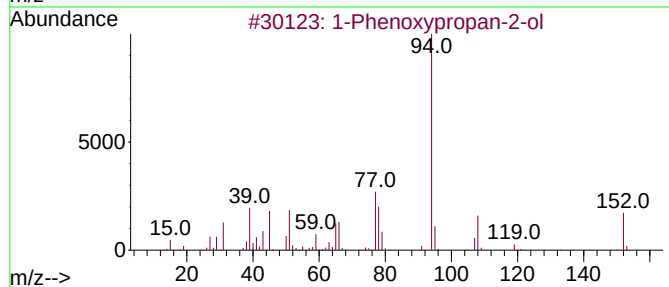
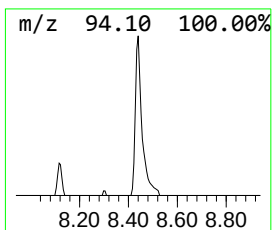
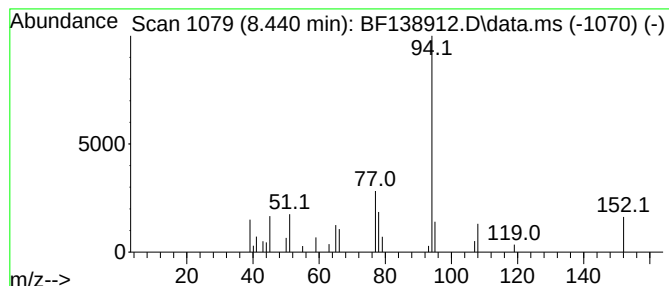
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.440	2.21 ng	34575	Naphthalene-d8	8.116

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	80
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5		2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	53



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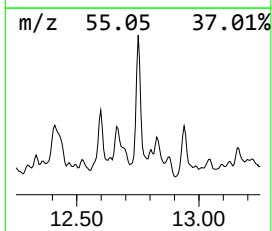
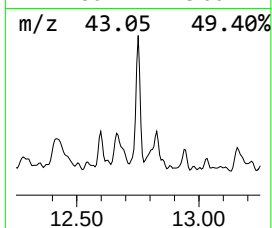
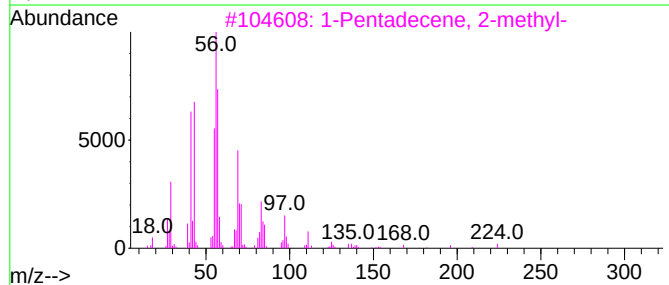
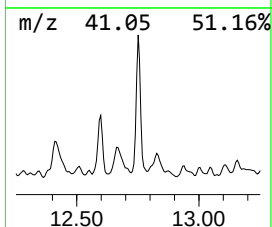
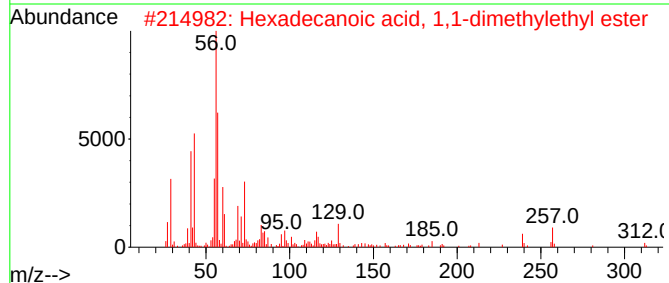
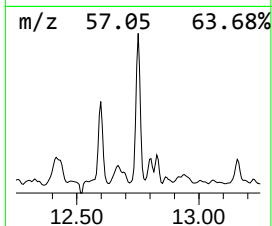
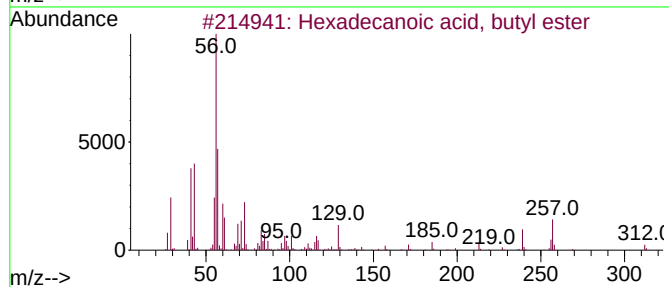
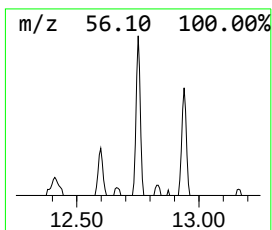
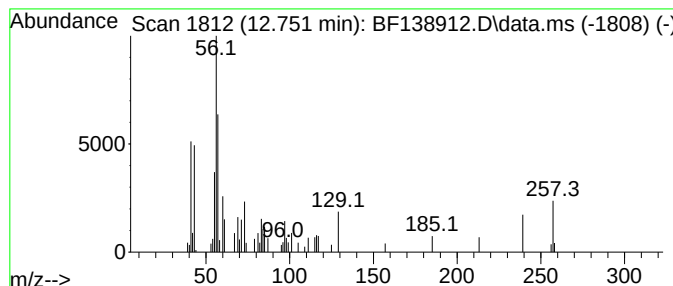
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	4.09 ng	36323	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3			1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	43
4			Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
5			Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	37



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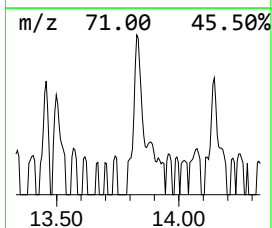
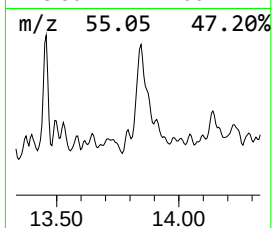
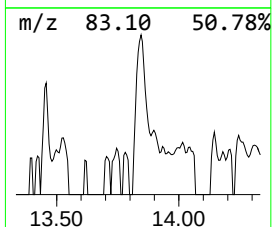
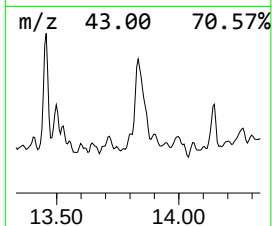
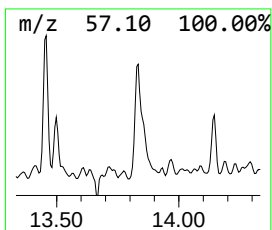
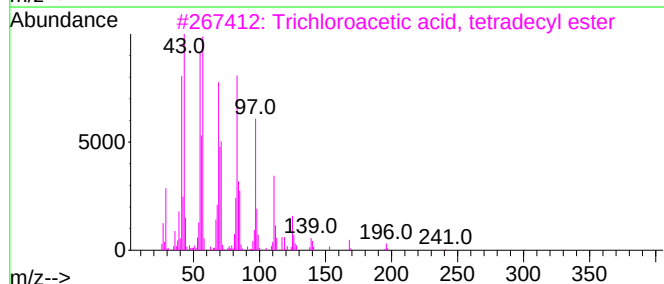
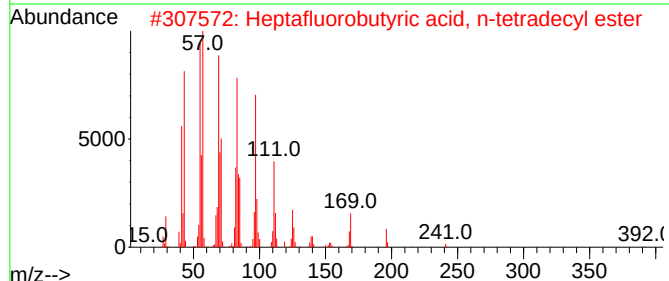
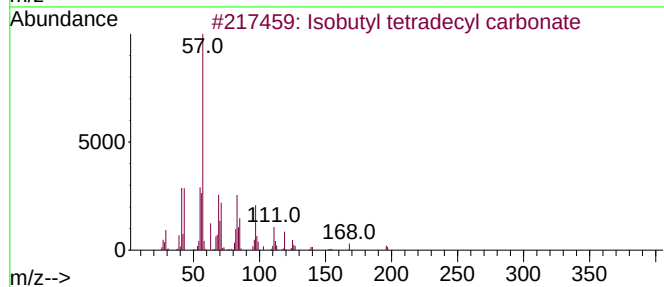
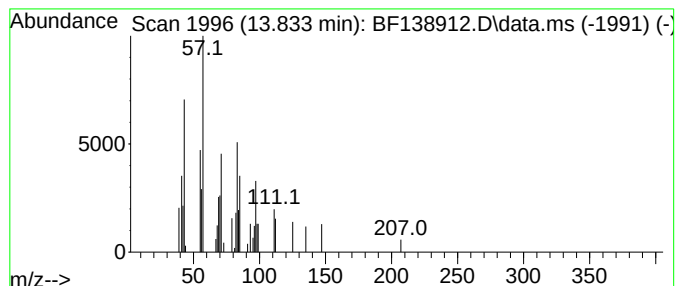
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Isobutyl tetradecyl carbonate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	3.35 ng	29804	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	72
2			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	64
3			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	62
4			1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	62
5			1-Octadecene	252	C18H36	000112-88-9	58



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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...	2.134	231.2	ng	2681460	1	6.840	232012	20.0
2-Pentanone, 4-...	5.063	8.0	ng	93007	1	6.840	232012	20.0
1-Phenoxypropan...	8.440	2.2	ng	34575	2	8.116	312451	20.0
Hexadecanoic ac...	12.751	4.1	ng	36323	5	13.998	177703	20.0
Isobutyl tetrad...	13.833	3.4	ng	29804	5	13.998	177703	20.0