

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081024\
 Data File : BF138917.D
 Acq On : 10 Aug 2024 18:53
 Operator : RC/JU
 Sample : P3466-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 924-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: BF138917.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	499	504	519	rVB	34751	53355	3.26%	0.681%
2	5.469	569	574	589	rBV	487107	664887	40.64%	8.486%
3	6.481	741	746	765	rVB	317951	435984	26.65%	5.564%
4	6.839	802	807	814	rBB	217488	267256	16.33%	3.411%
5	7.404	897	903	915	rBV	708387	938074	57.34%	11.973%
6	8.122	1019	1025	1043	rBB	279274	362799	22.17%	4.630%
7	8.433	1074	1078	1095	rVB	40878	61283	3.75%	0.782%
8	9.192	1201	1207	1212	rBV	1312977	1636116	100.00%	20.882%
9	9.869	1317	1322	1332	rVB	313165	400478	24.48%	5.111%
10	9.963	1332	1338	1344	rBV	38058	54804	3.35%	0.699%
11	10.251	1383	1387	1392	rBV	20386	24706	1.51%	0.315%
12	10.663	1452	1457	1471	rBV	694588	905855	55.37%	11.561%
13	11.304	1562	1566	1570	rVB	15451	17266	1.06%	0.220%
14	11.357	1570	1575	1584	rBV	292015	362941	22.18%	4.632%
15	11.880	1659	1664	1681	rBV3	11683	23516	1.44%	0.300%
16	12.398	1747	1752	1768	rVB2	9705	21950	1.34%	0.280%
17	12.939	1838	1844	1849	rBV	877056	1096466	67.02%	13.994%
18	13.827	1989	1995	2006	rBV	17499	35737	2.18%	0.456%
19	13.998	2020	2024	2033	rVB	151853	195090	11.92%	2.490%
20	14.821	2159	2164	2171	rBV	20464	29432	1.80%	0.376%
21	15.462	2267	2273	2284	rBV	156004	247175	15.11%	3.155%

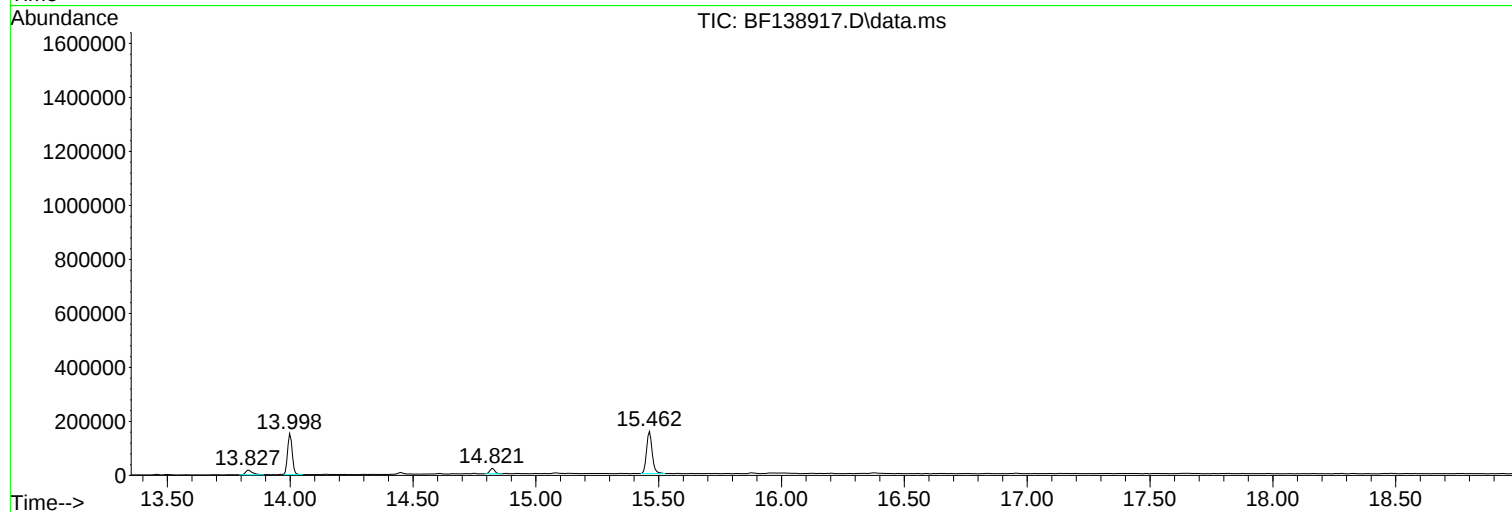
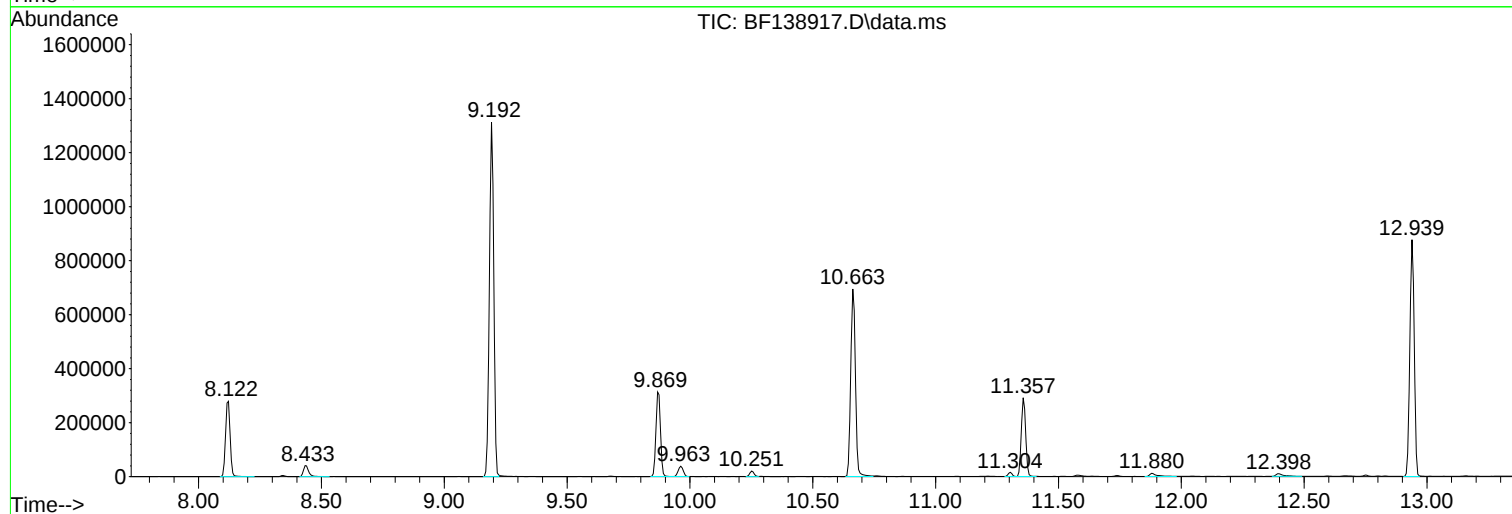
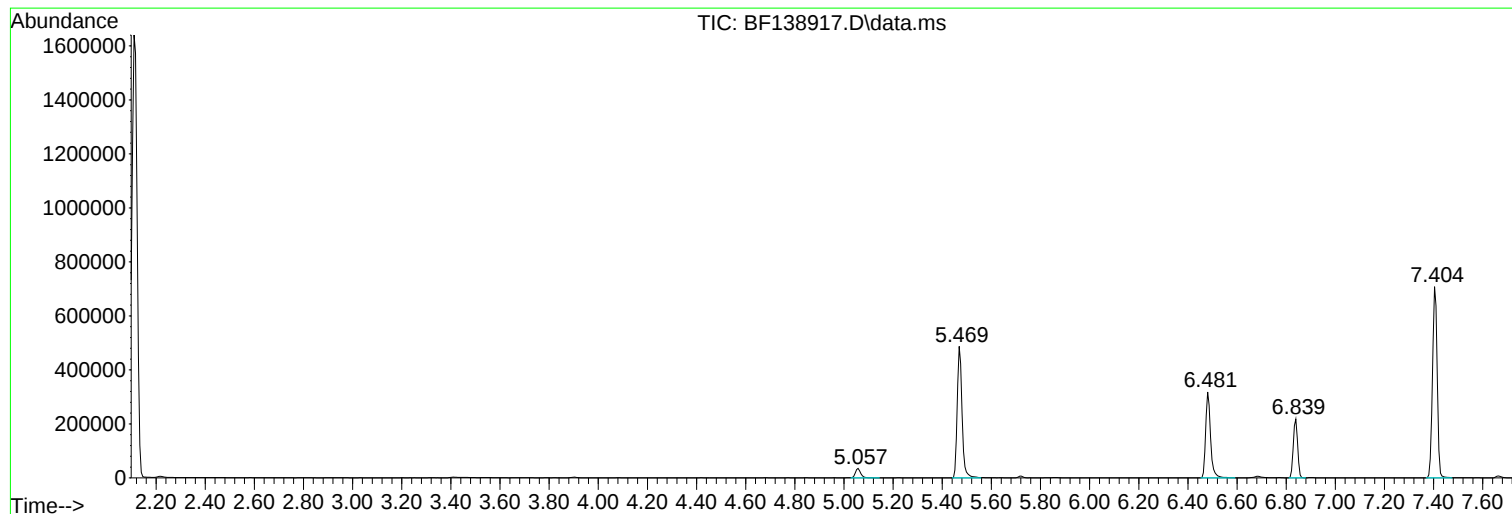
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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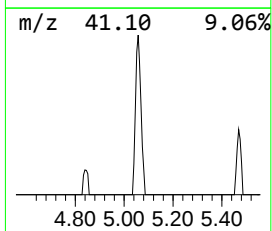
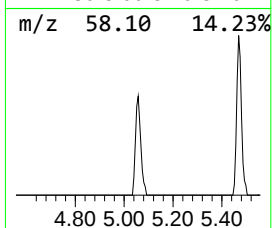
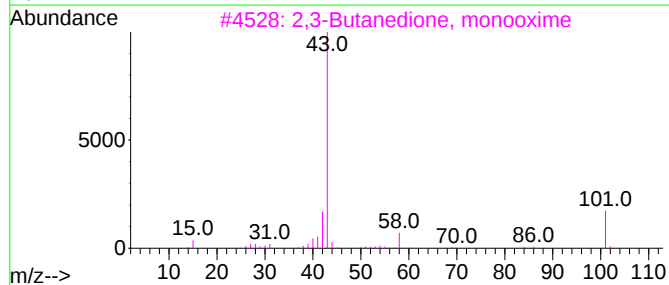
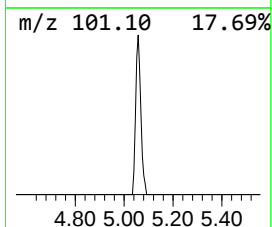
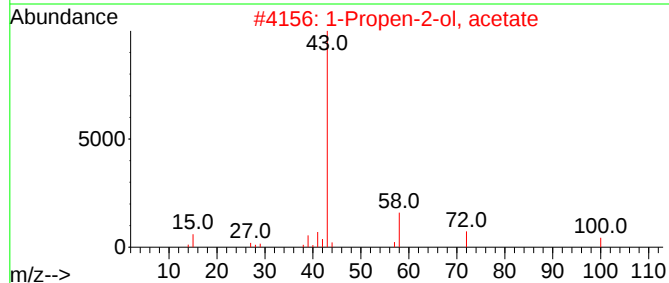
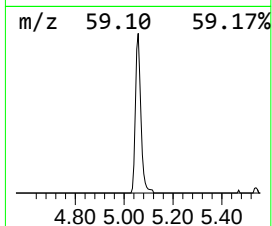
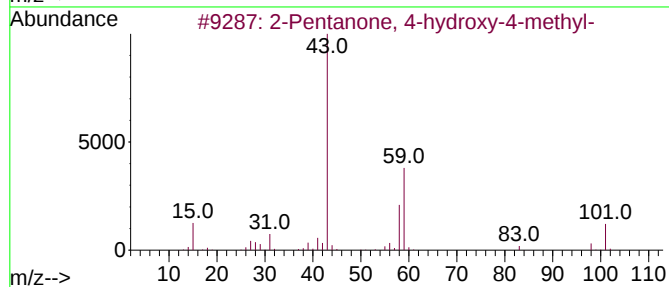
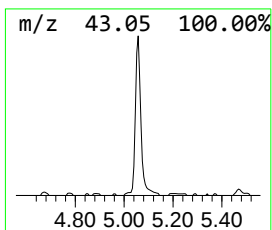
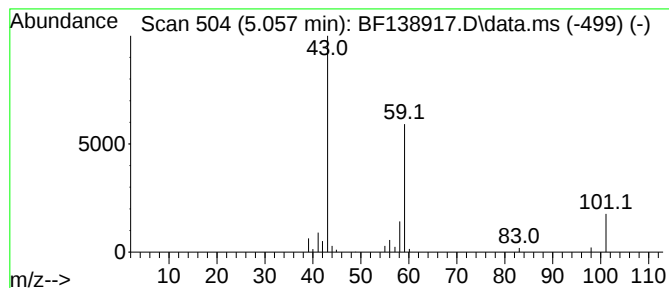
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	3.99 ng	53355	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9		



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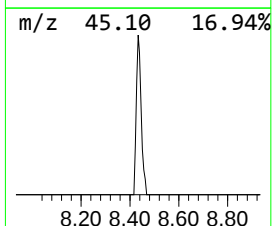
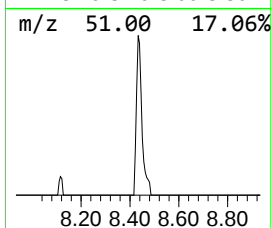
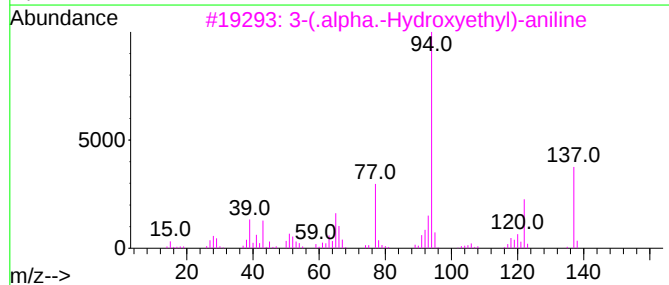
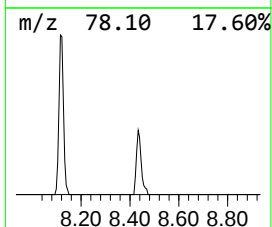
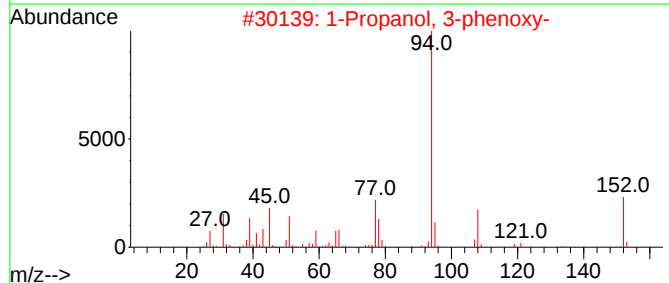
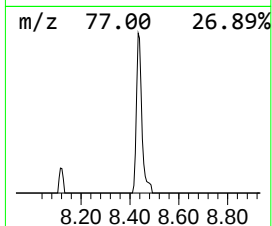
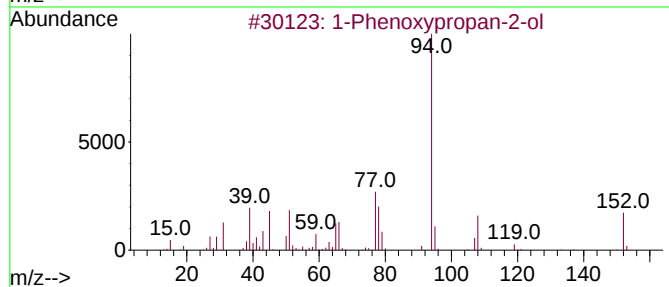
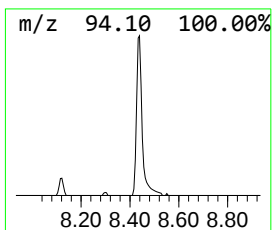
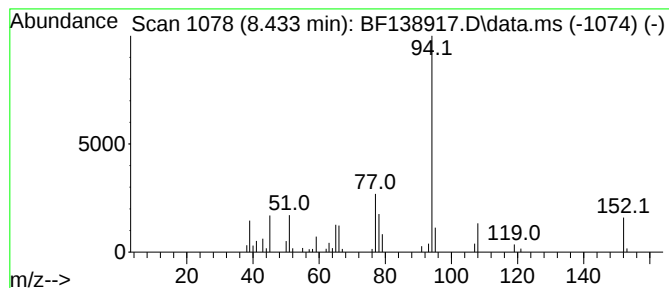
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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	3.38 ng	61283	Naphthalene-d8	8.122

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	81
3		3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	64
4		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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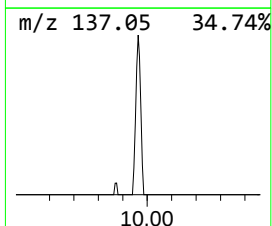
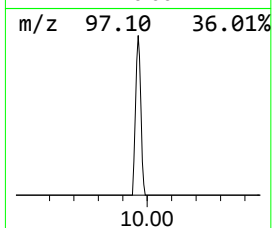
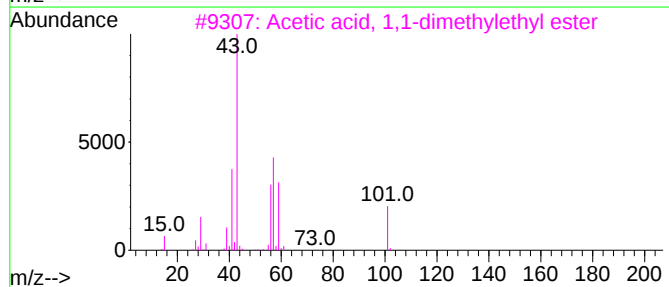
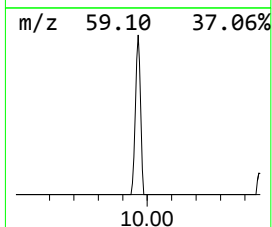
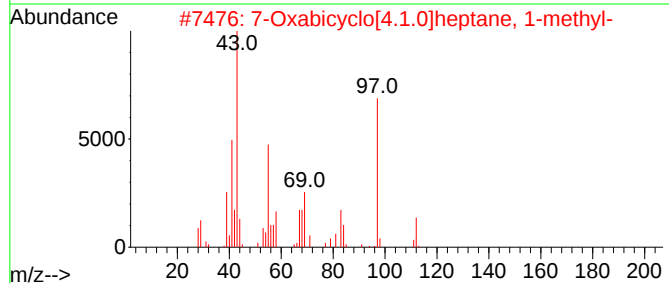
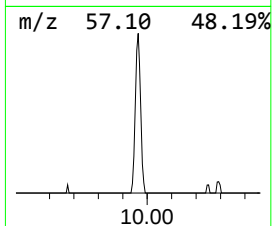
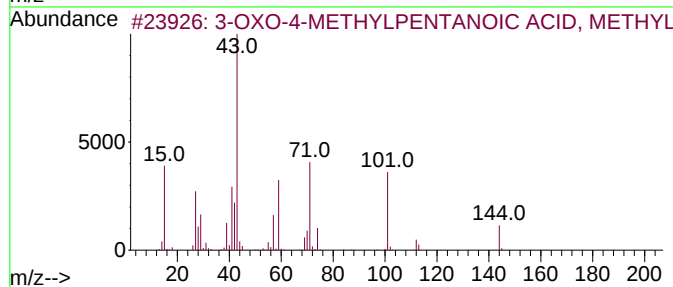
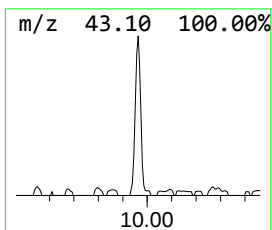
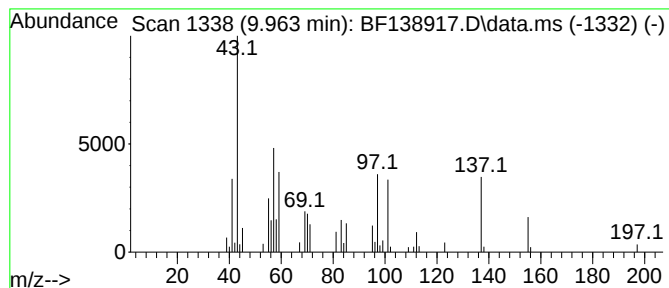
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown9.963 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.963	2.74 ng	54804	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	12
2			7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	10
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
4			Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10
5			3-Octanol, acetate	172	C10H20O2	004864-61-3	10



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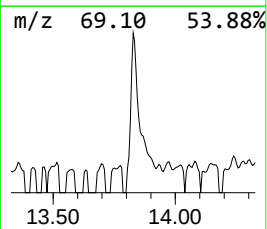
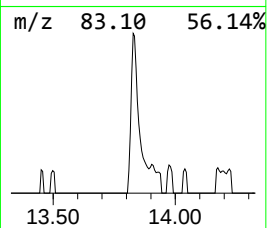
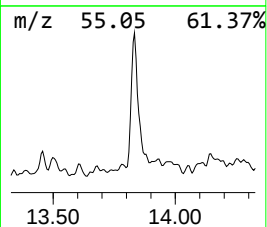
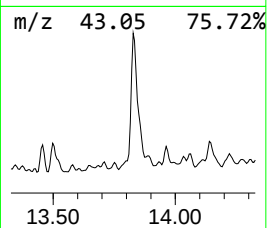
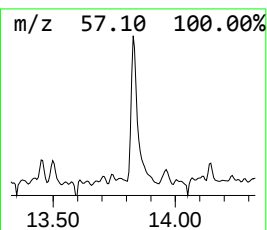
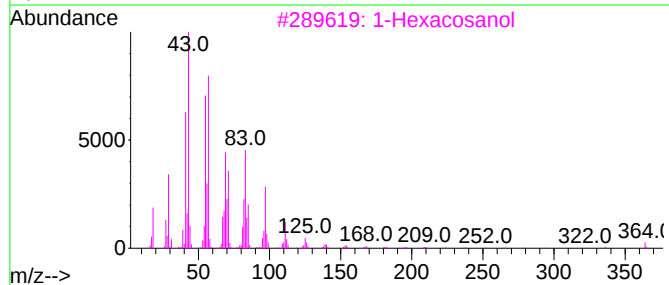
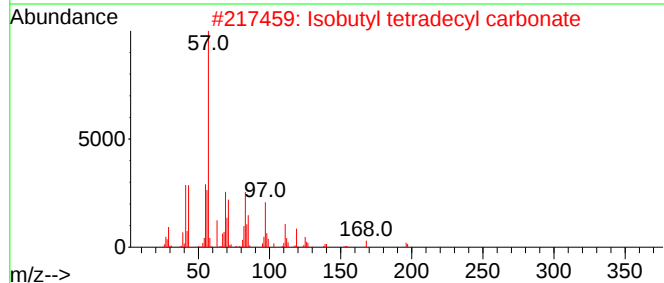
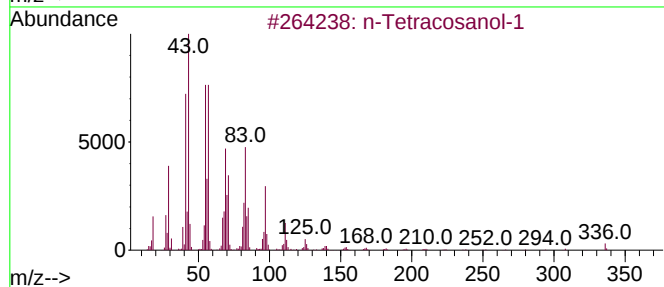
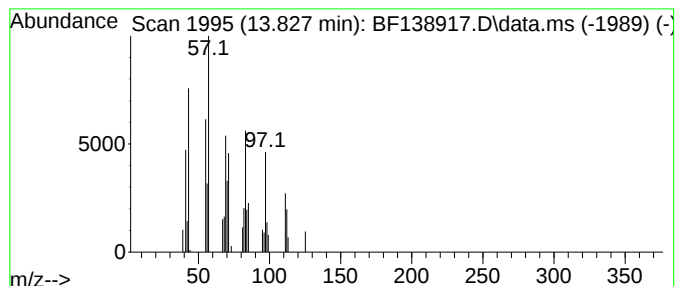
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Tetracosanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	3.66 ng	35737	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	74
2			Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	72
3			1-Hexacosanol	382	C26H54O	000506-52-5	38
4			Octane, 4-ethyl-	142	C10H22	015869-86-0	35
5			6-Methyl-1,7-diazabicyclo[4.1.0]...	112	C6H12N2	108602-71-7	30



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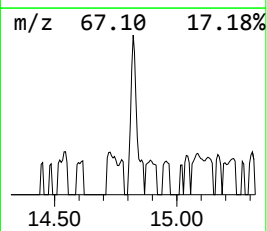
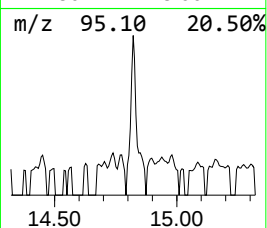
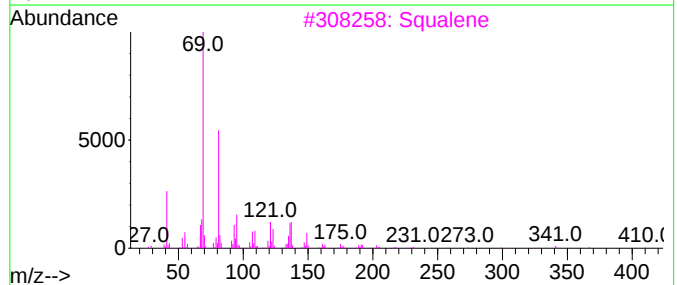
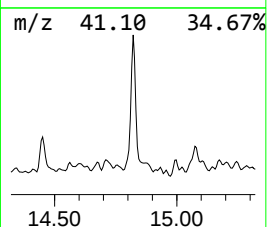
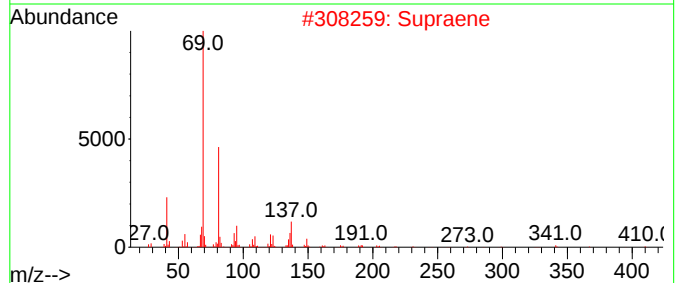
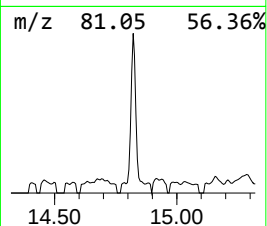
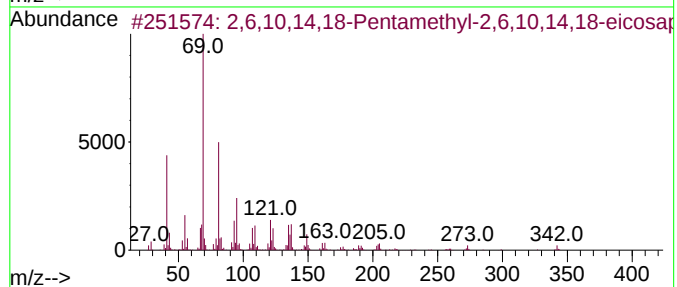
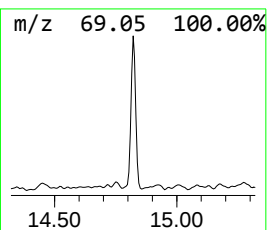
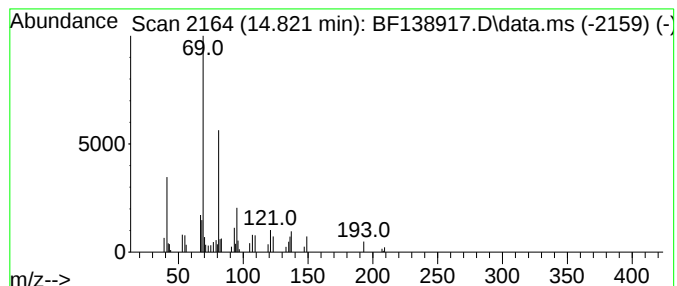
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Peak Number 5 2,6,10,14,18-Pentamethyl-2,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.821	2.38 ng	29432	Perylene-d12	15.462	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
2	Supraene	410	C30H50	007683-64-9	72
3	Squalene	410	C30H50	000111-02-4	72
4	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	64
5	(2E,6E)-3,7,11-Trimethyldodeca-2...	376	C25H44O2	078368-57-7	59



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.057	4.0	ng	53355	1	6.839	267256	20.0
1-Phenoxypropan...	8.433	3.4	ng	61283	2	8.122	362799	20.0
unknown9.963	9.963	2.7	ng	54804	3	9.869	400478	20.0
n-Tetracosanol-1	13.827	3.7	ng	35737	5	13.998	195090	20.0
2,6,10,14,18-Pe...	14.821	2.4	ng	29432	6	15.462	247175	20.0