

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031423\
 Data File : BF132785.D
 Acq On : 14 Mar 2023 18:53
 Operator : CG\JU
 Sample : 01894-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C0AA9

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132785.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.598	338	342	349	rBV	136477	164537	2.38%	0.454%
2	5.198	439	444	453	rBV	1172959	1322857	19.10%	3.651%
3	5.593	507	511	530	rBV	2721348	2681501	38.72%	7.401%
4	5.981	573	577	587	rBV	225910	198837	2.87%	0.549%
5	6.592	677	681	699	rBV	1857738	1717882	24.80%	4.741%
6	6.963	741	744	748	rBV	1497921	1193149	17.23%	3.293%
7	7.534	836	841	844	rBV	3799306	3854221	55.65%	10.637%
8	8.245	959	962	966	rBV	1651806	1406155	20.30%	3.881%
9	9.328	1141	1146	1149	rBV	6140376	6107382	88.18%	16.856%
10	10.004	1258	1261	1265	rBV	1939436	1657527	23.93%	4.575%
11	10.722	1379	1383	1387	rVB	431383	337317	4.87%	0.931%
12	10.804	1392	1397	1400	rBV	4608094	4255990	61.45%	11.746%
13	11.498	1511	1515	1519	rBV	2105131	1826747	26.37%	5.042%
14	13.092	1781	1786	1789	rBV	7058788	6926096	100.00%	19.116%
15	13.968	1932	1935	1945	rBV	100045	147591	2.13%	0.407%
16	14.157	1963	1967	1976	rVB	1148369	1170771	16.90%	3.231%
17	14.998	2106	2110	2114	rBV2	83246	88116	1.27%	0.243%
18	15.686	2222	2227	2240	rVB	918136	1175797	16.98%	3.245%

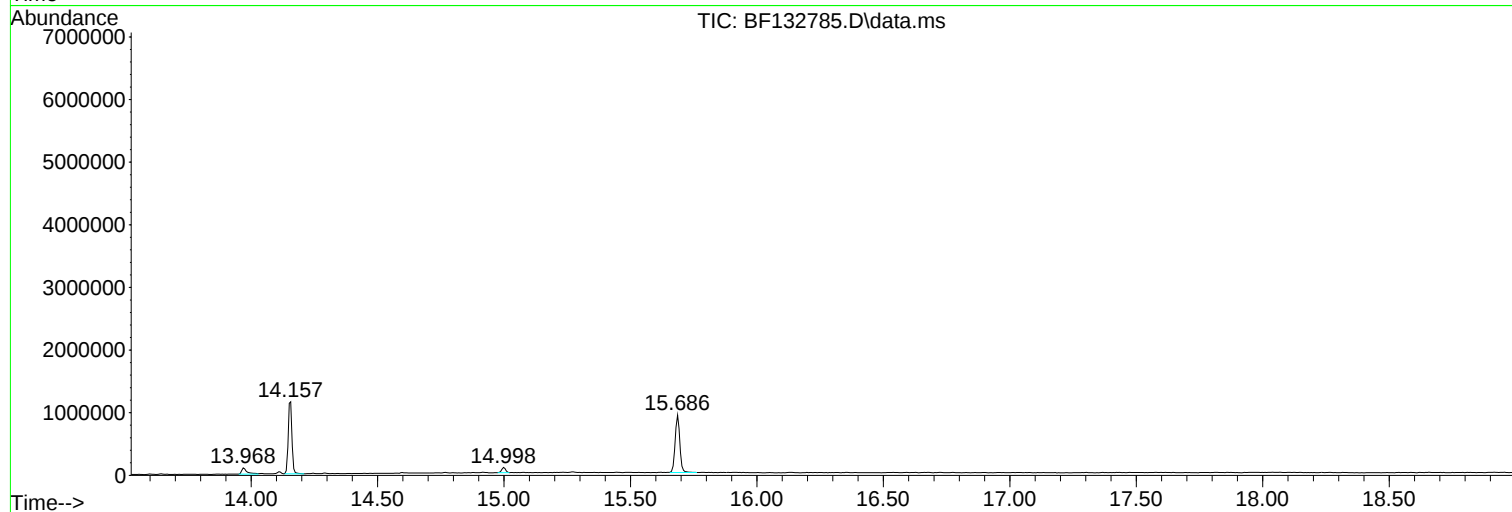
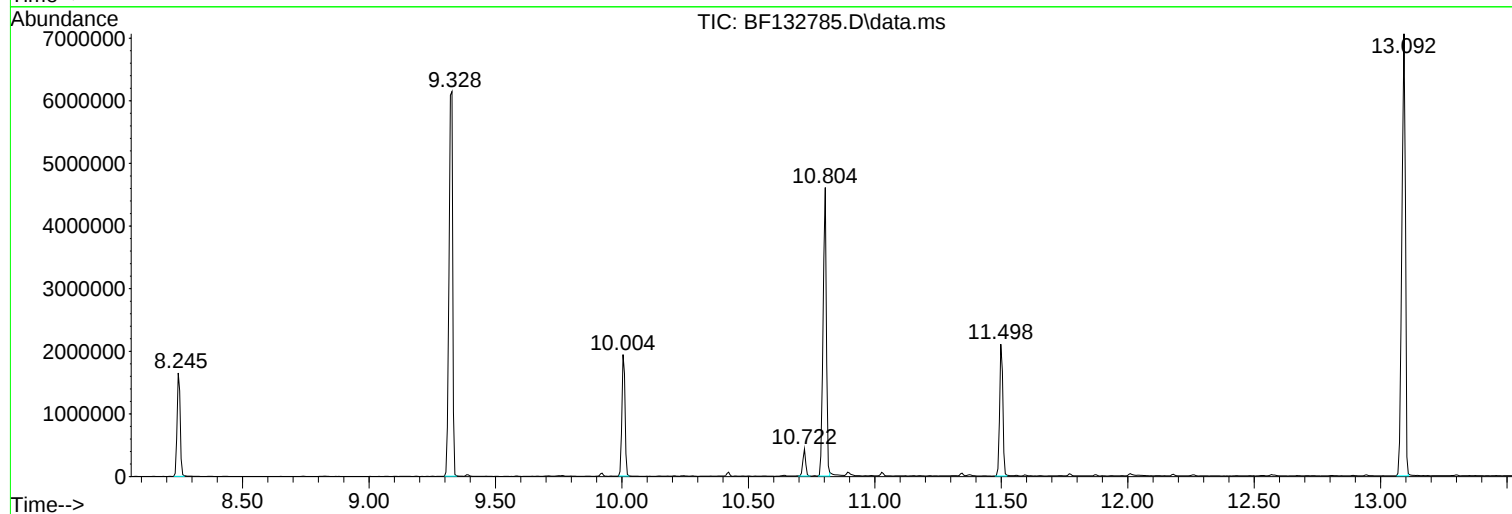
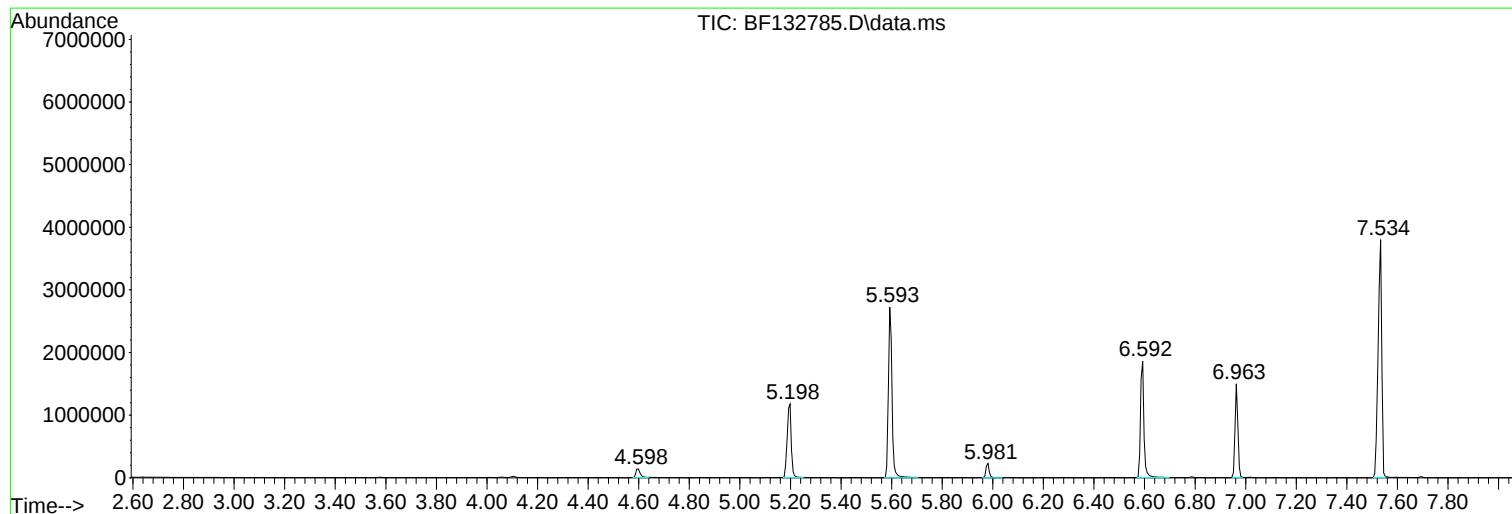
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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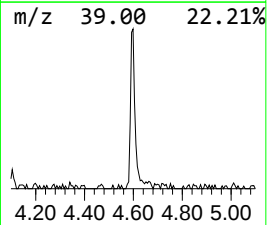
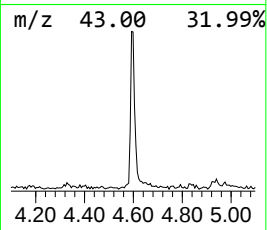
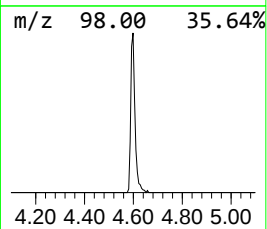
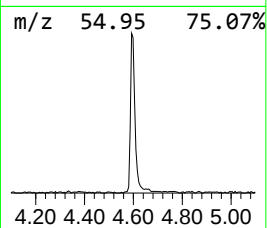
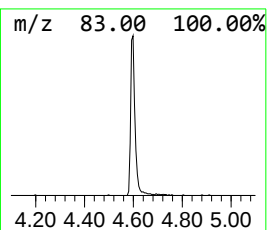
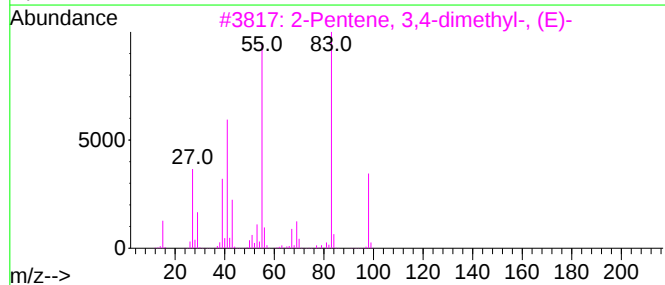
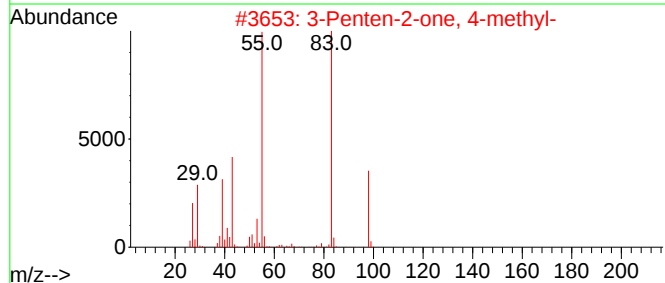
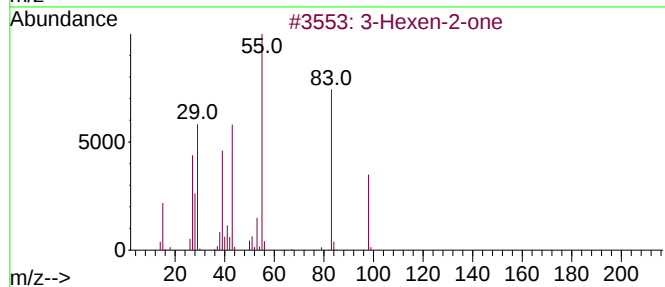
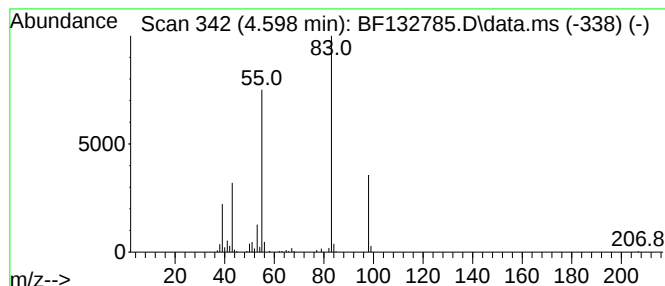
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.598	2.76 ng	164537	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
4			2,4-Azetidinedione, 3,3-diethyl-	141	C7H11N02	042282-85-9	78
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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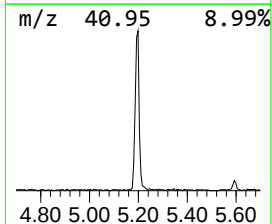
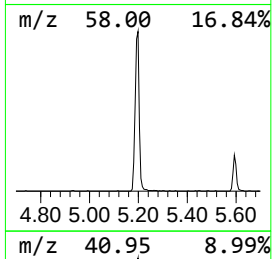
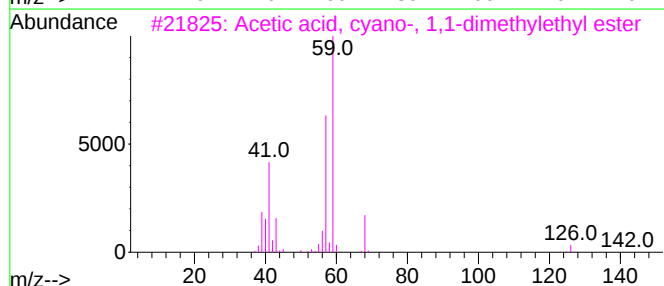
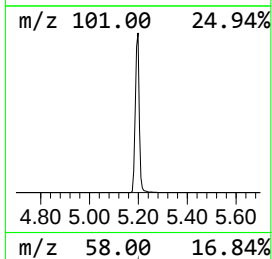
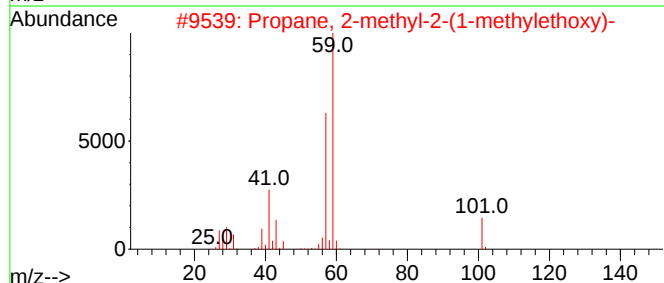
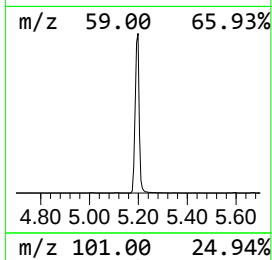
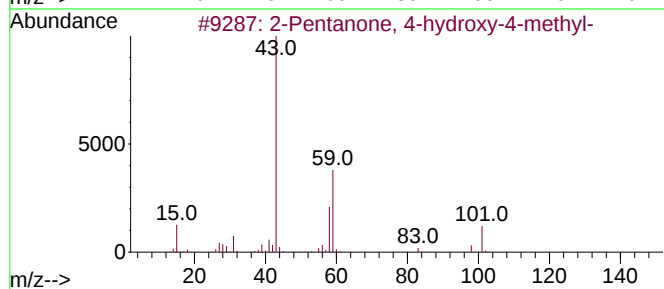
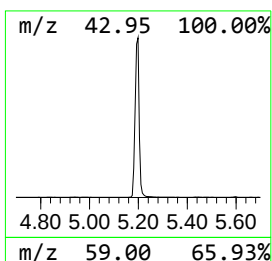
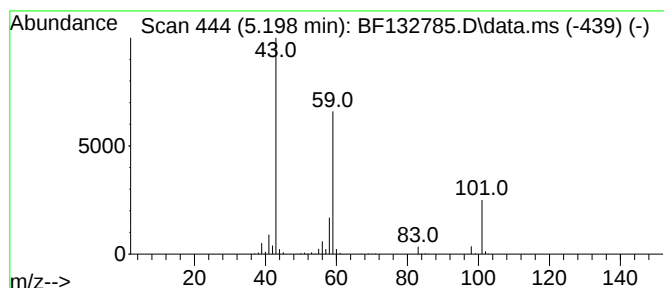
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.198	22.17 ng	1322860	1,4-Dichlorobenzene-d4	6.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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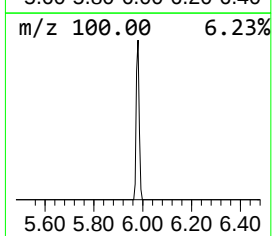
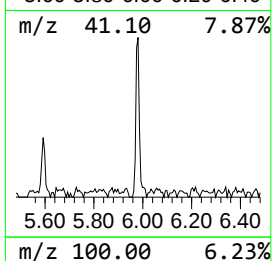
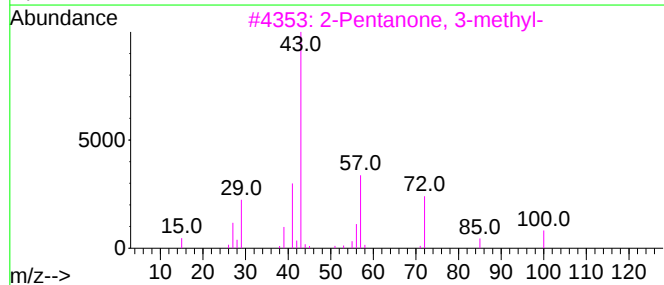
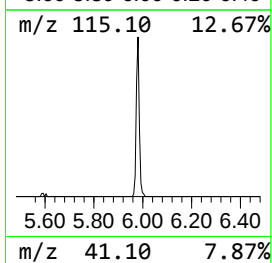
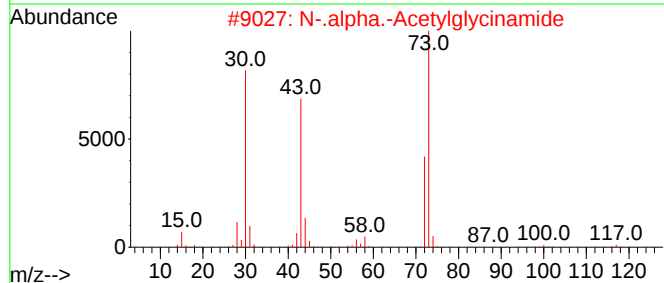
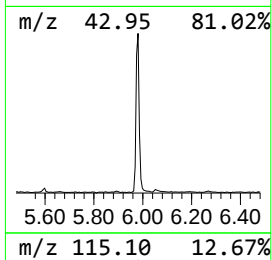
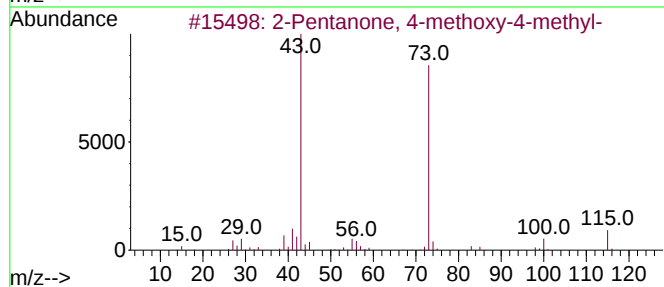
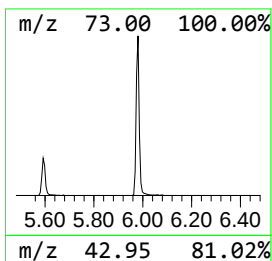
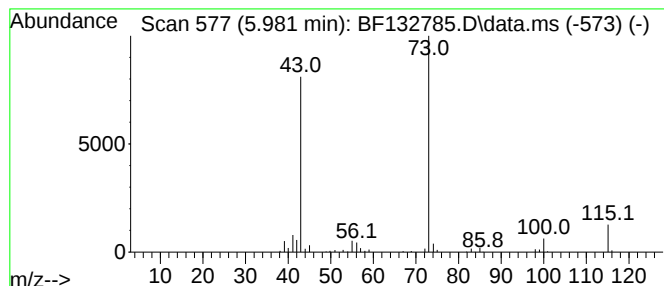
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.981	3.33 ng	198837	1,4-Dichlorobenzene-d4	6.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	25
3		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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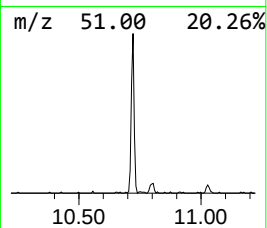
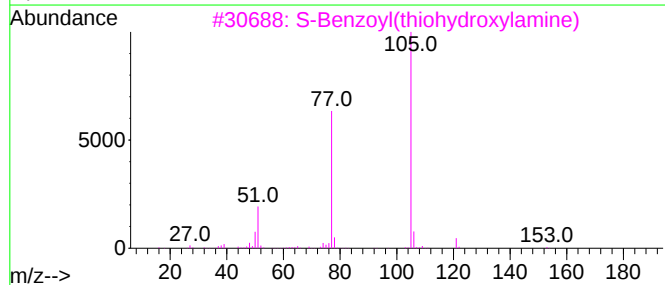
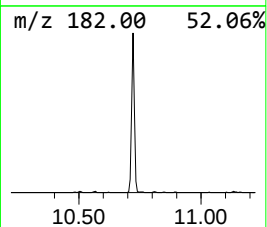
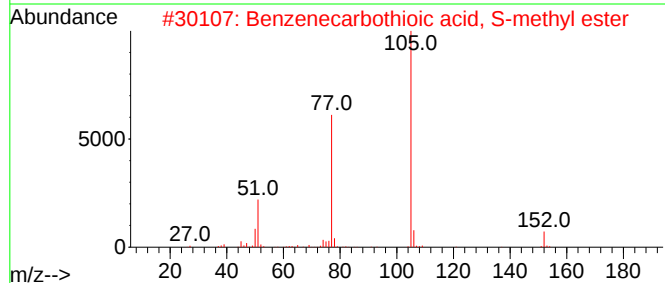
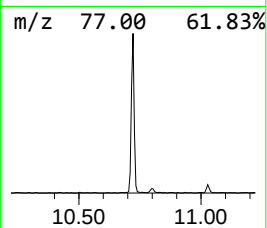
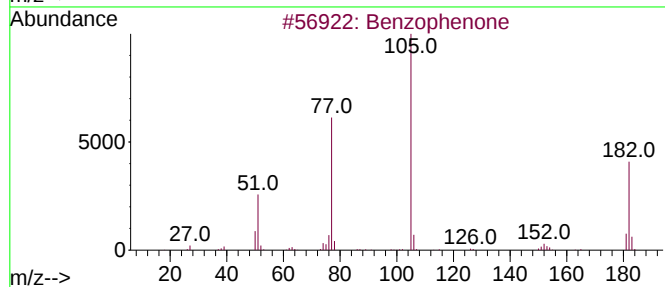
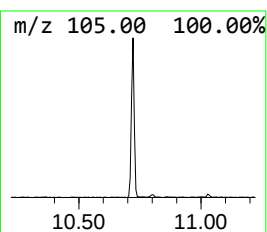
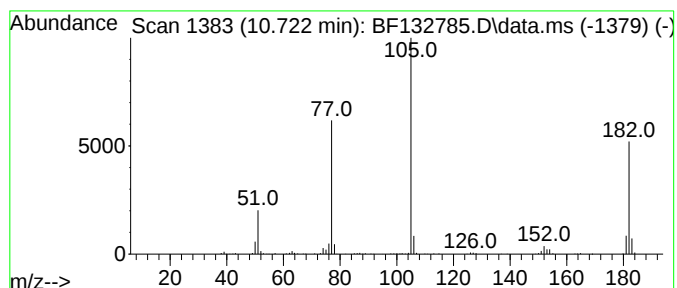
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Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.722	4.07 ng	337317	Acenaphthene-d10	10.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47



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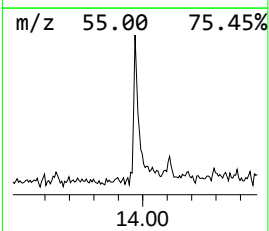
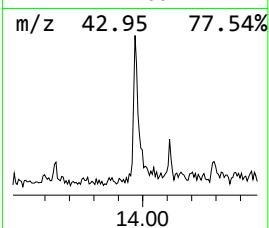
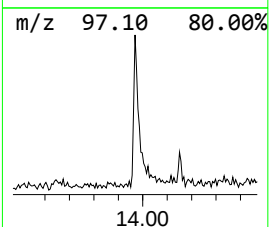
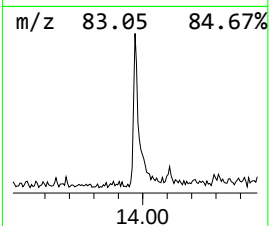
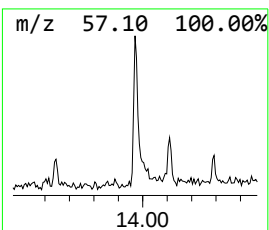
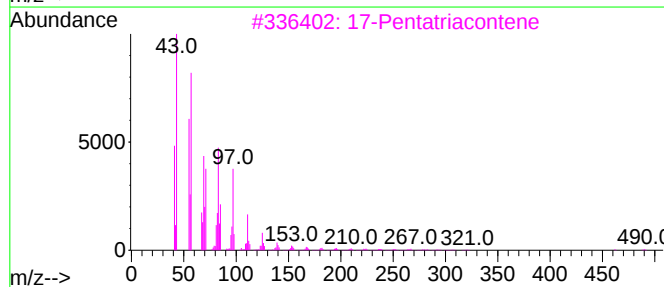
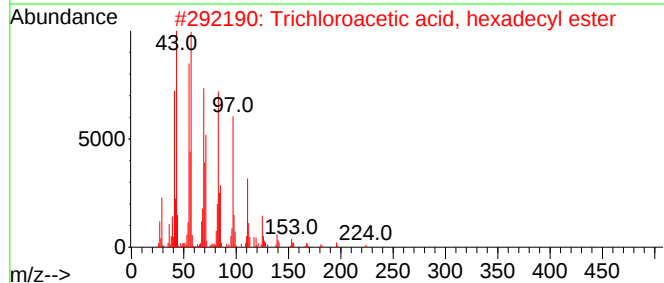
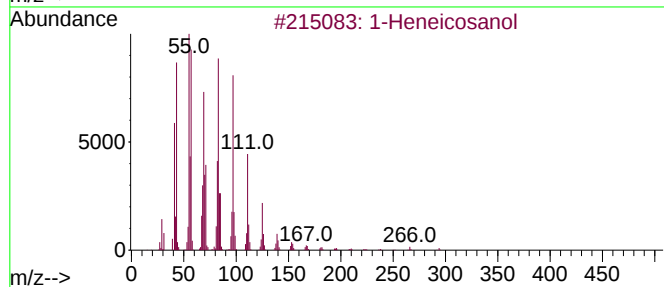
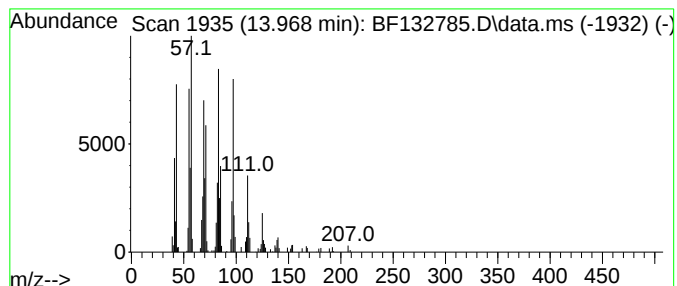
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.968	2.52 ng	147591	Chrysene-d12	14.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			17-Pentatriacontene	491	C35H70	006971-40-0	91
4			1-Hexacosanol	382	C26H54O	000506-52-5	90
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90



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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
3-Hexen-2-one	4.598	2.8	ng	164537	1	6.963	1193150	20.0
2-Pentanone, 4-...	5.198	22.2	ng	1322860	1	6.963	1193150	20.0
2-Pentanone, 4-...	5.981	3.3	ng	198837	1	6.963	1193150	20.0
Benzophenone	10.722	4.1	ng	337317	3	10.004	1657530	20.0
1-Heneicosanol	13.968	2.5	ng	147591	5	14.157	1170770	20.0