

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111124\
 Data File : BE101572.D
 Acq On : 11 Nov 2024 15:08
 Operator : RC/JU
 Sample : P4796-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_E
 ClientSampleId :
 TP-4

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_E\Methods\8270-BE110624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BE101572.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.673	10	14	28	rVV	1205599	1388688	48.47%	9.890%
2	2.861	42	46	54	rBV	195553	239489	8.36%	1.706%
3	4.776	369	372	389	rVB	27870	48863	1.71%	0.348%
4	5.305	456	462	485	rBV	362408	624968	21.82%	4.451%
5	6.932	732	739	765	rBV	347878	681515	23.79%	4.854%
6	7.555	838	845	854	rBV	117960	188015	6.56%	1.339%
7	8.765	1040	1051	1066	rBV	232500	420823	14.69%	2.997%
8	10.322	1308	1316	1331	rBV	157348	288356	10.07%	2.054%
9	12.784	1728	1735	1757	rBV	763533	1197252	41.79%	8.527%
10	14.165	1963	1970	1983	rBV	288475	451643	15.77%	3.217%
11	15.534	2197	2203	2214	rBV	155149	217742	7.60%	1.551%
12	15.675	2220	2227	2251	rBV	777368	1213047	42.34%	8.640%
13	16.903	2429	2436	2451	rBV	435887	639950	22.34%	4.558%
14	19.494	2871	2877	2894	rBV	2232390	2864787	100.00%	20.403%
15	21.063	3139	3144	3155	rVV	664814	868138	30.30%	6.183%
16	21.744	3255	3260	3270	rVB	1366294	1644703	57.41%	11.714%
17	22.320	3355	3358	3364	rVB2	21129	30685	1.07%	0.219%
18	23.348	3525	3533	3541	rBV	514665	1032039	36.02%	7.350%

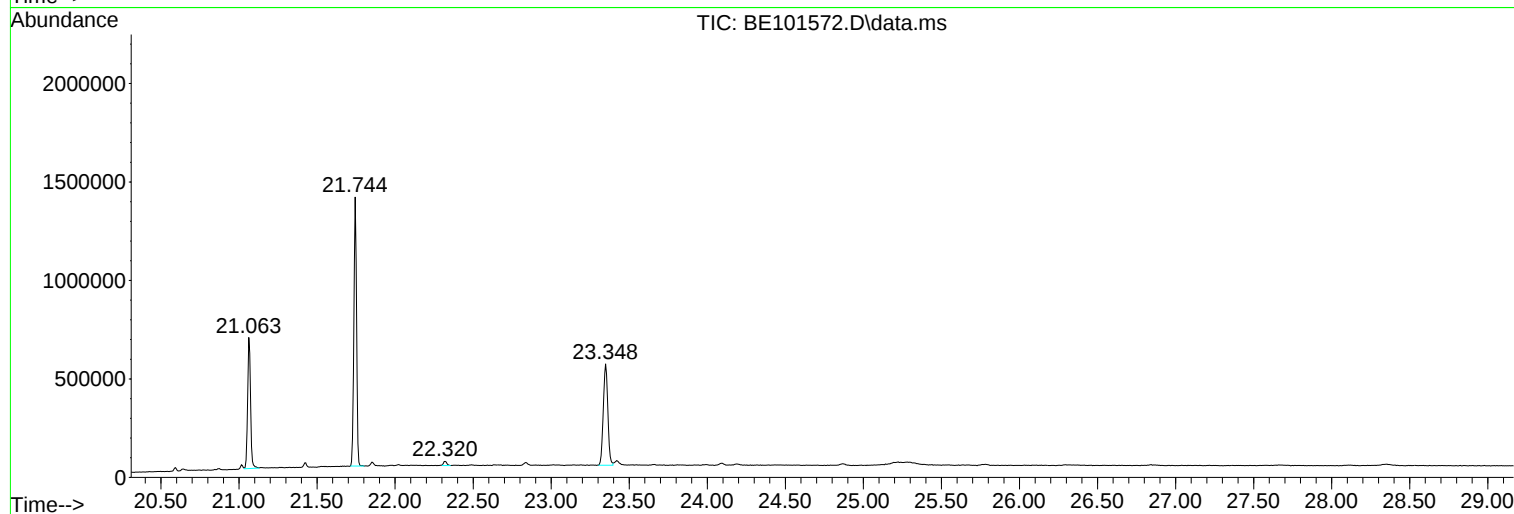
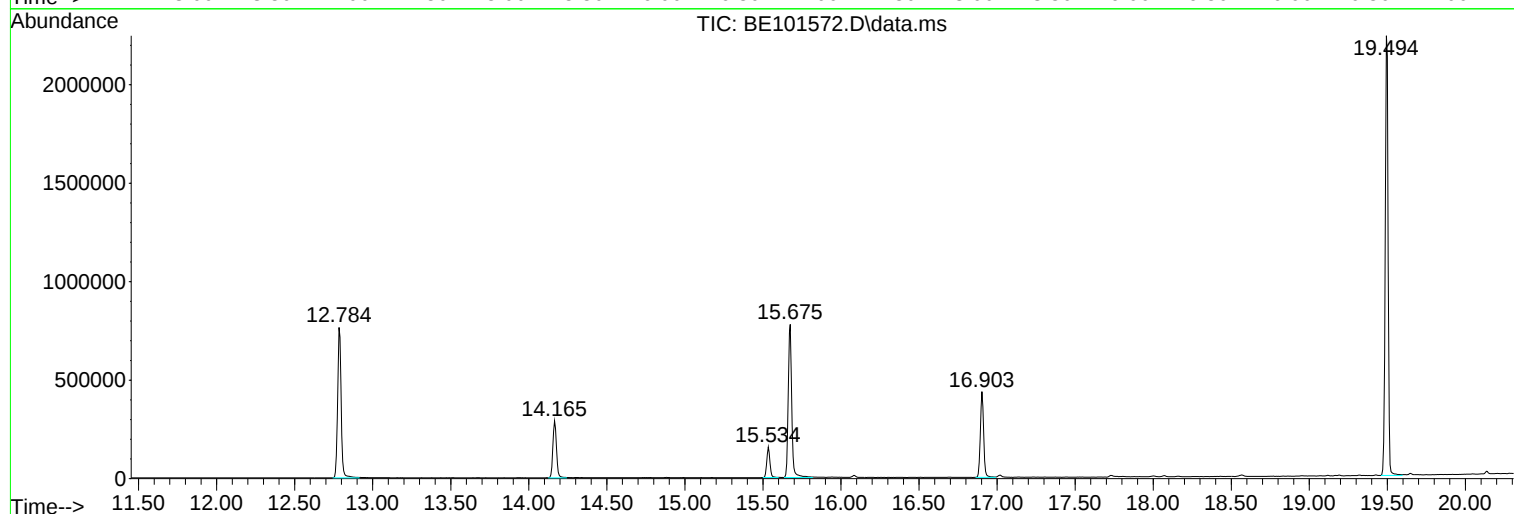
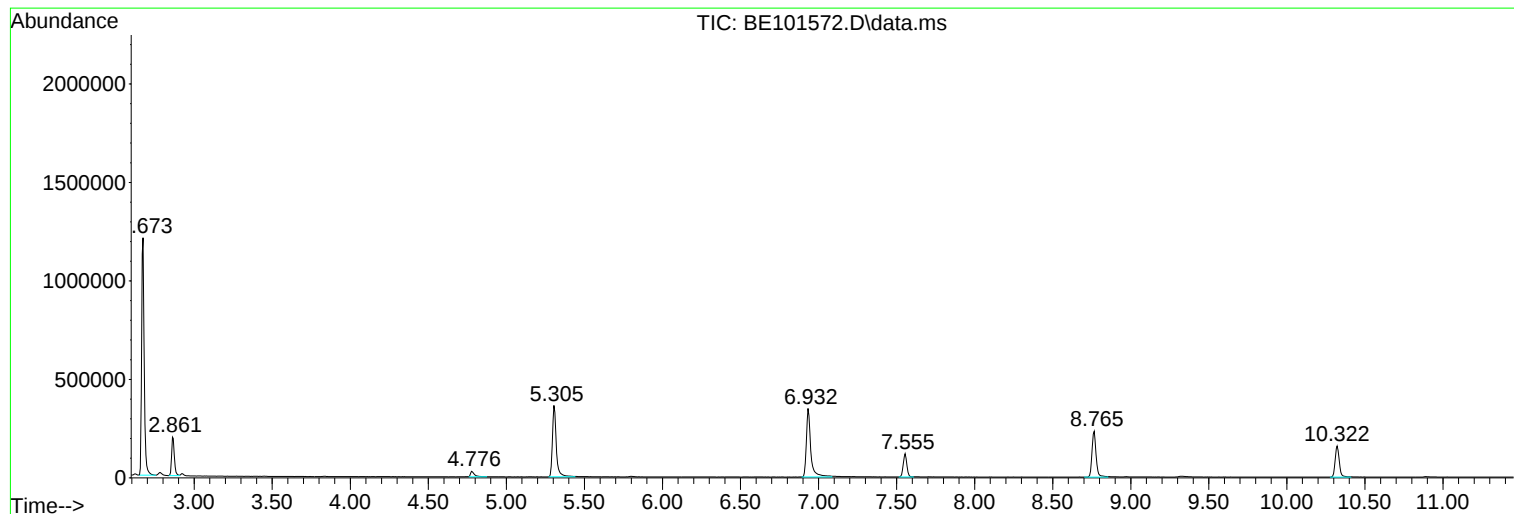
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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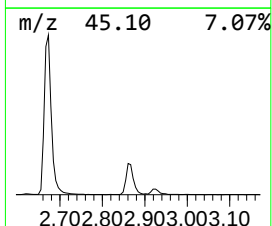
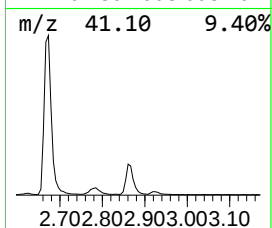
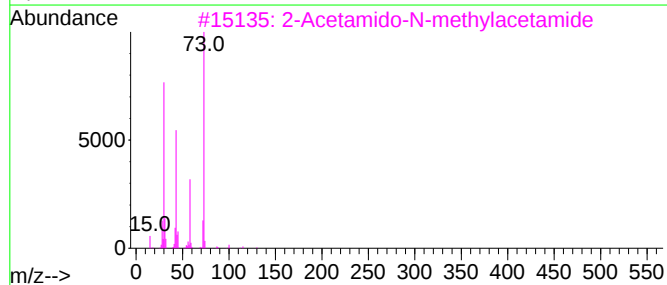
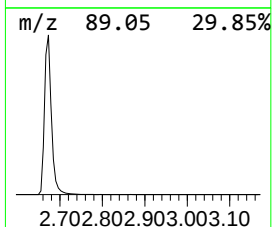
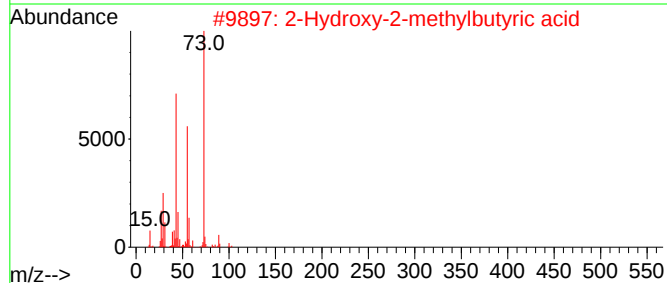
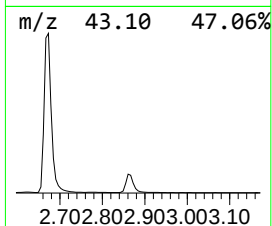
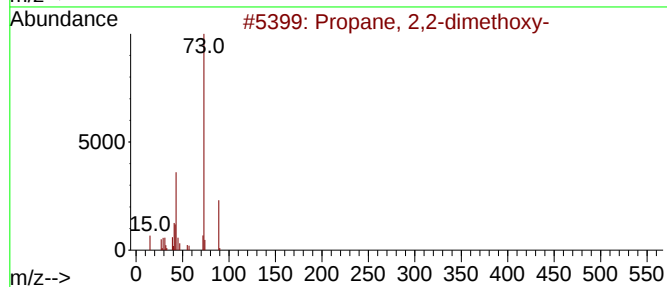
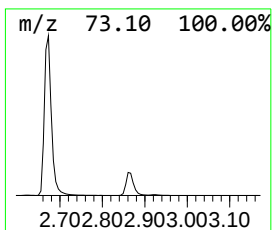
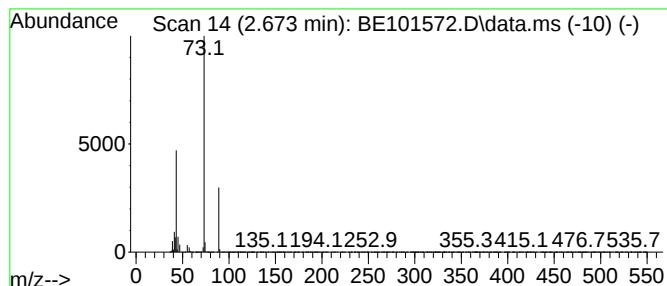
Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.673	147.72 ng	1388690	1,4-Dichlorobenzene-d4	7.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9
4			1,3-Dioxolane, 2-hexyl-	158	C9H18O2	001708-34-5	9
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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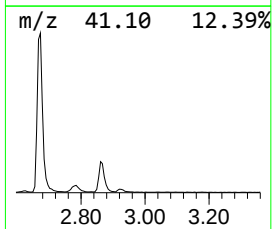
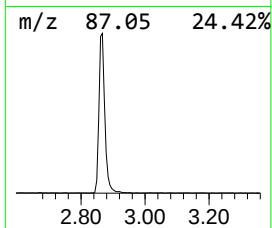
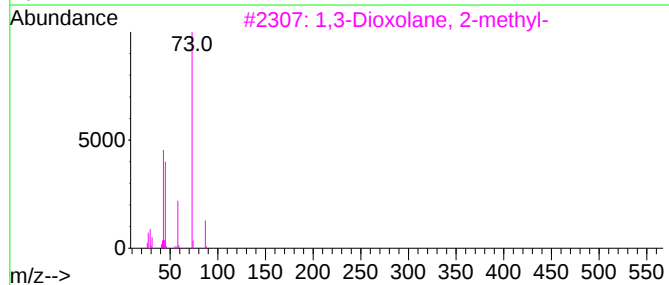
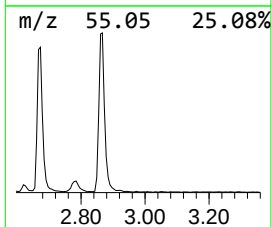
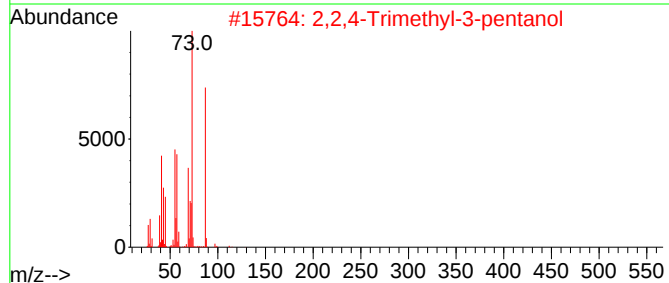
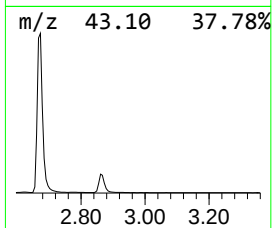
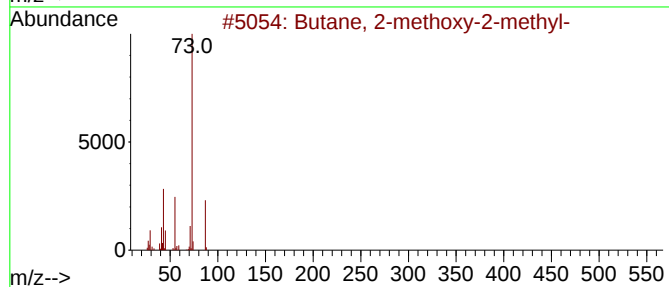
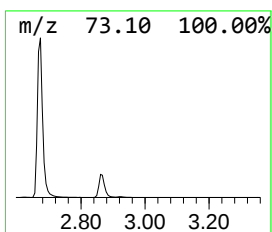
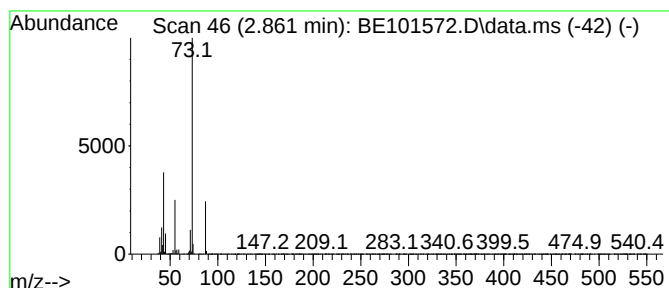
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.861	25.48 ng	239489	1,4-Dichlorobenzene-d4	7.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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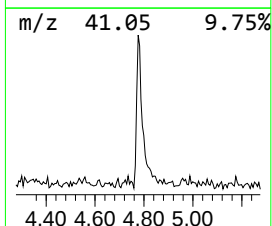
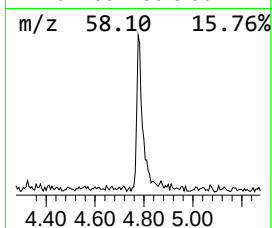
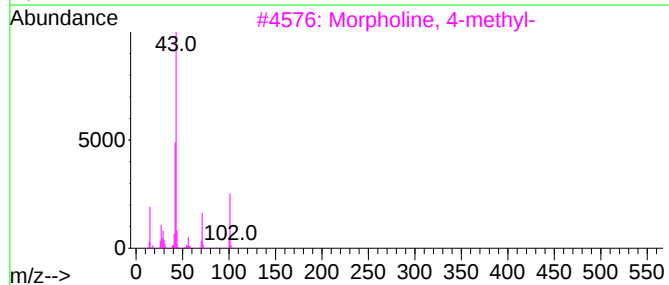
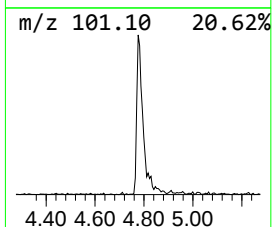
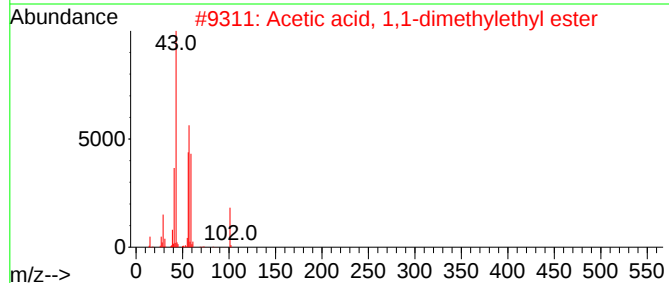
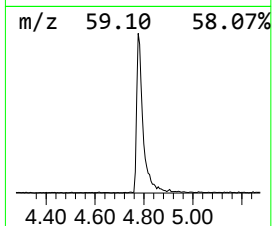
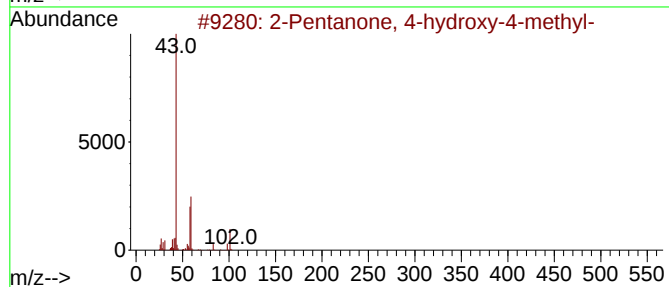
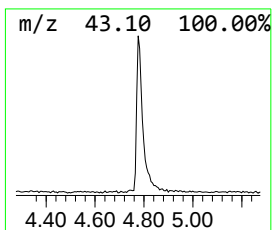
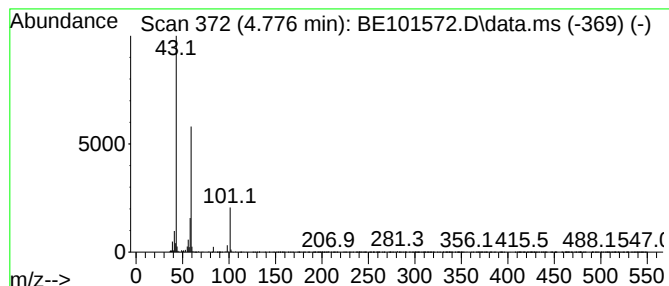
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.776	5.20 ng	48863	1,4-Dichlorobenzene-d4	7.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Hexanamide	115	C6H13NO	000628-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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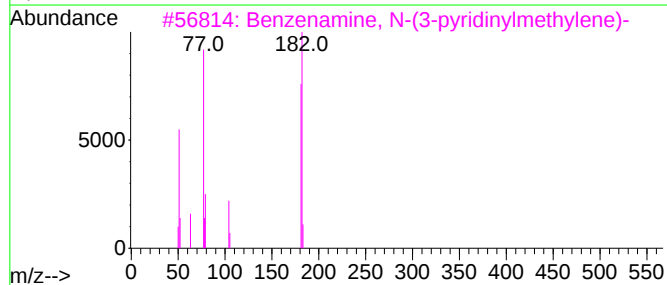
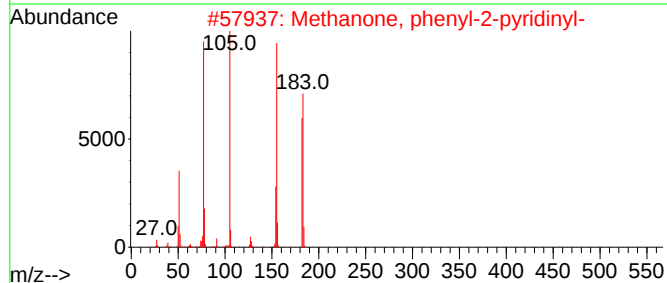
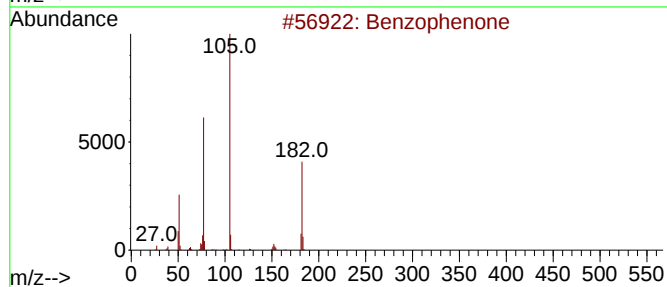
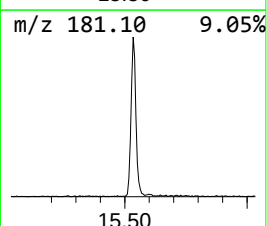
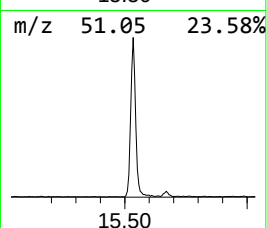
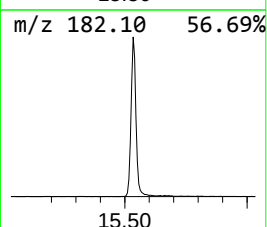
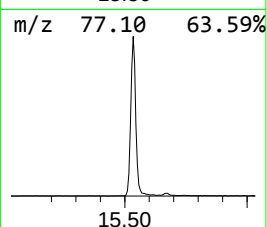
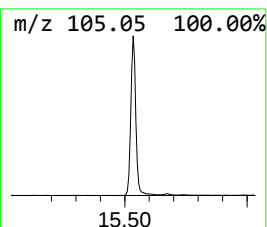
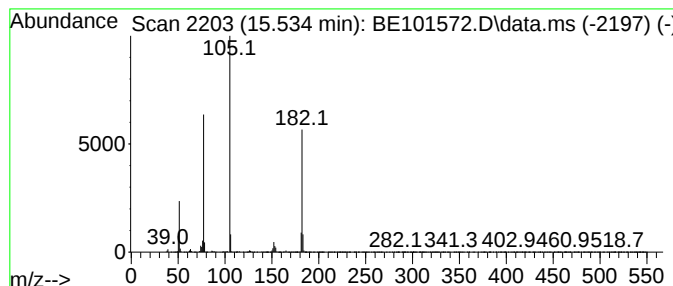
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.534	6.80 ng	217742	Phenanthrene-d10	16.903

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	56
3			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	42
4			Azobenzene	182	C12H10N2	000103-33-3	40
5			2,3-Dihydro-1-oxo-1H-phenalene	182	C13H10O	000518-85-4	27



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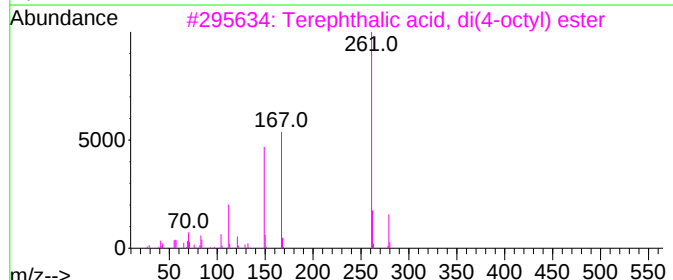
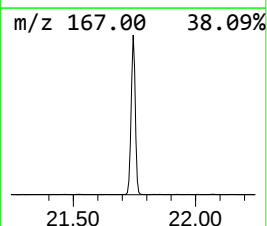
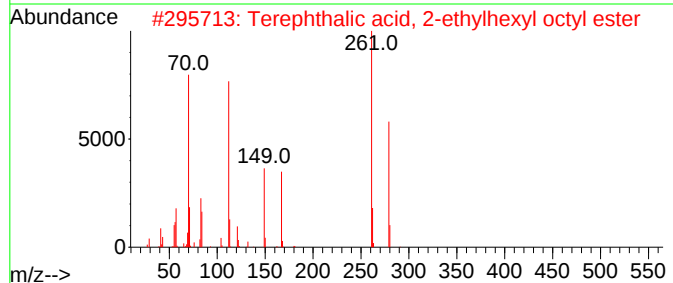
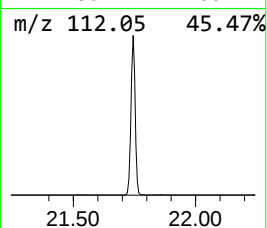
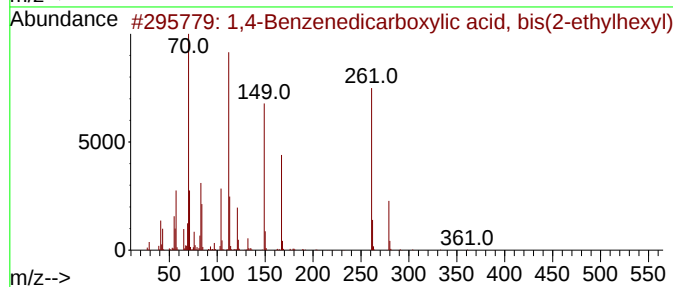
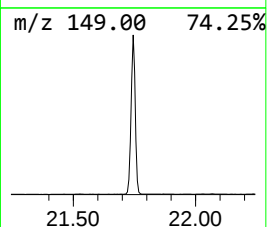
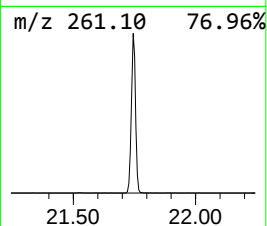
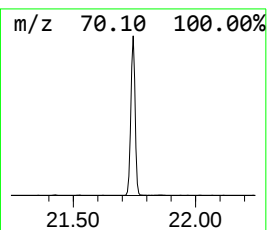
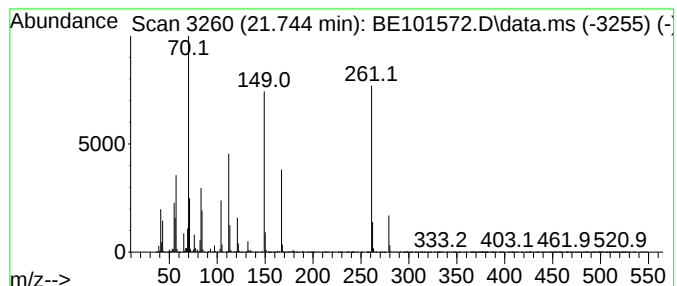
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Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.744	37.89 ng	1644700	Chrysene-d12	21.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	90
2			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	50
3			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	50
4			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	49
5			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-di...	2.673	147.7	ng	1388690	1	7.555	188015	20.0
Butane, 2-metho...	2.861	25.5	ng	239489	1	7.555	188015	20.0
2-Pentanone, 4-...	4.776	5.2	ng	48863	1	7.555	188015	20.0
Benzophenone	15.534	6.8	ng	217742	4	16.903	639950	20.0
1,4-Benzenedica...	21.744	37.9	ng	1644700	5	21.063	868138	20.0