

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
 Data File : BF133899.D
 Acq On : 22 Jun 2023 13:55
 Operator : CG\JU
 Sample : 03321-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-25

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133899.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	20	rVB	357351	457336	24.33%	3.068%
2	2.234	22	25	31	rVB2	21523	31752	1.69%	0.213%
3	4.475	403	406	413	rBV2	17394	22123	1.18%	0.148%
4	5.092	505	511	522	rBV	688816	823688	43.81%	5.526%
5	5.492	574	579	582	rBV	1825283	1631425	86.78%	10.945%
6	5.881	641	645	650	rBV	44713	38104	2.03%	0.256%
7	6.492	744	749	752	rBV	1863648	1659867	88.29%	11.136%
8	6.857	808	811	815	rBV	758958	583436	31.03%	3.914%
9	7.416	902	906	910	rBV	1223653	1107893	58.93%	7.433%
10	8.139	1025	1029	1032	rBV	860274	735758	39.14%	4.936%
11	9.216	1208	1212	1215	rBV	2238754	1879967	100.00%	12.612%
12	9.892	1324	1327	1331	rBV	869146	771764	41.05%	5.178%
13	10.610	1446	1449	1458	rBV	423147	338294	17.99%	2.270%
14	10.686	1458	1462	1472	rBV	1362972	1151299	61.24%	7.724%
15	10.922	1499	1502	1506	rBV	70229	56617	3.01%	0.380%
16	11.386	1577	1581	1588	rBV	822658	710408	37.79%	4.766%
17	11.916	1668	1671	1685	rBV2	165606	183646	9.77%	1.232%
18	12.710	1802	1806	1810	rBV3	31321	40808	2.17%	0.274%
19	12.986	1848	1853	1856	rBV	1486593	1392802	74.09%	9.344%
20	13.904	2005	2009	2016	rBV5	62481	147239	7.83%	0.988%
21	14.045	2029	2033	2041	rVB	683573	607251	32.30%	4.074%
22	14.215	2059	2062	2072	rBV8	20305	43011	2.29%	0.289%
23	15.551	2285	2289	2294	rBV	382799	491473	26.14%	3.297%

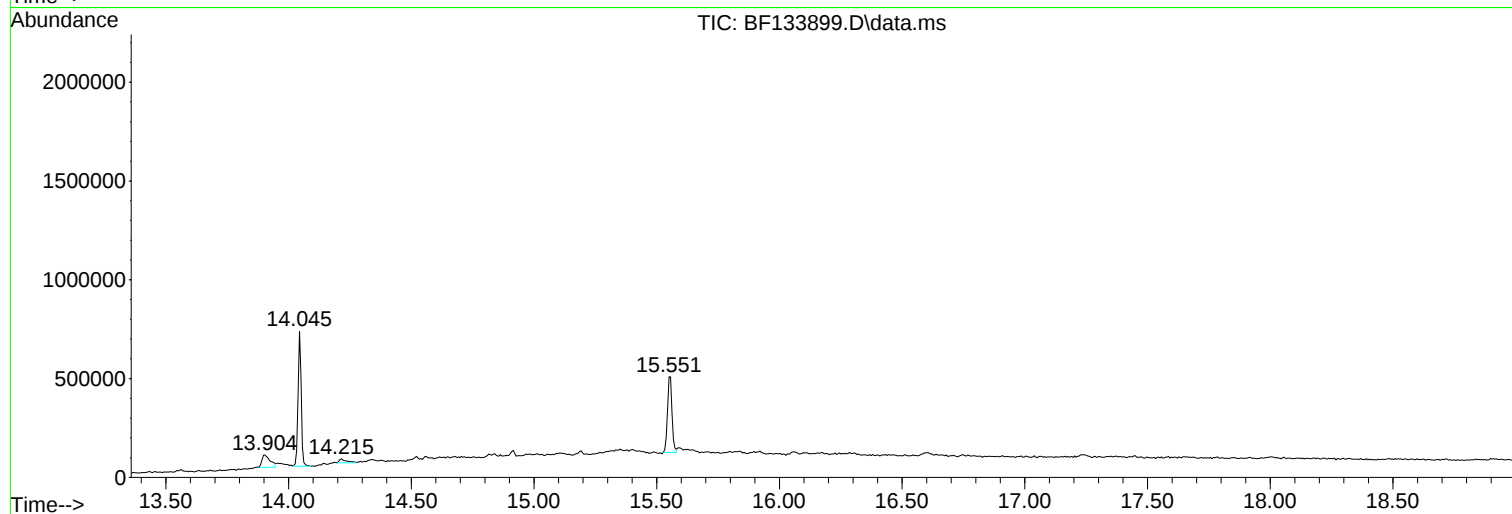
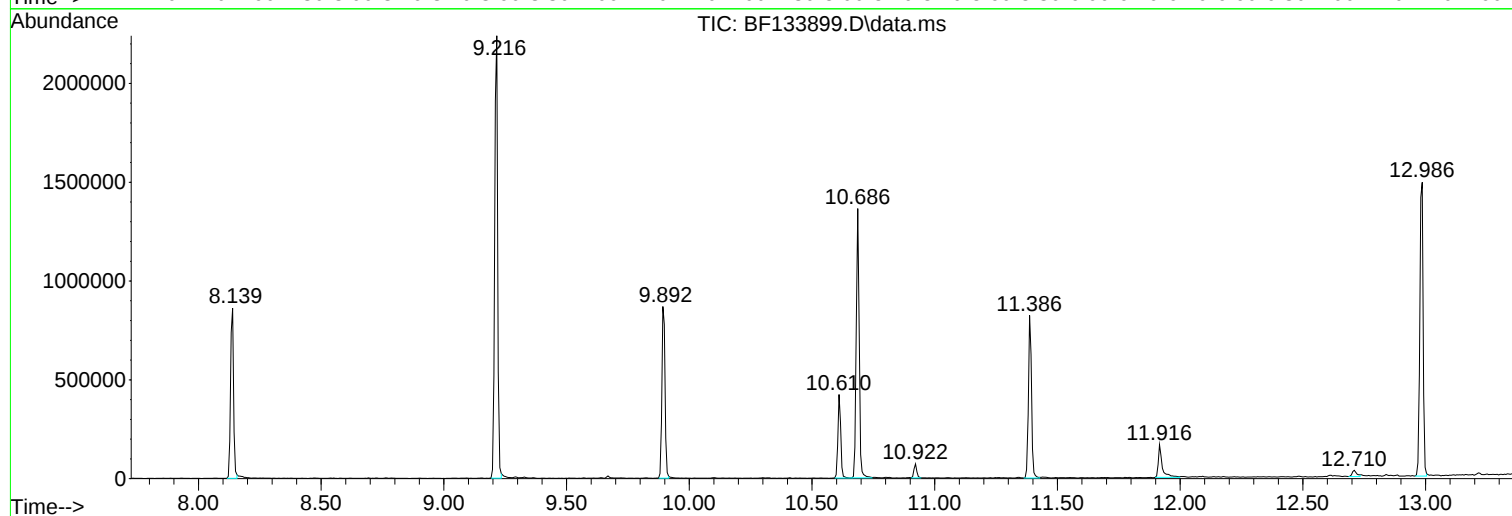
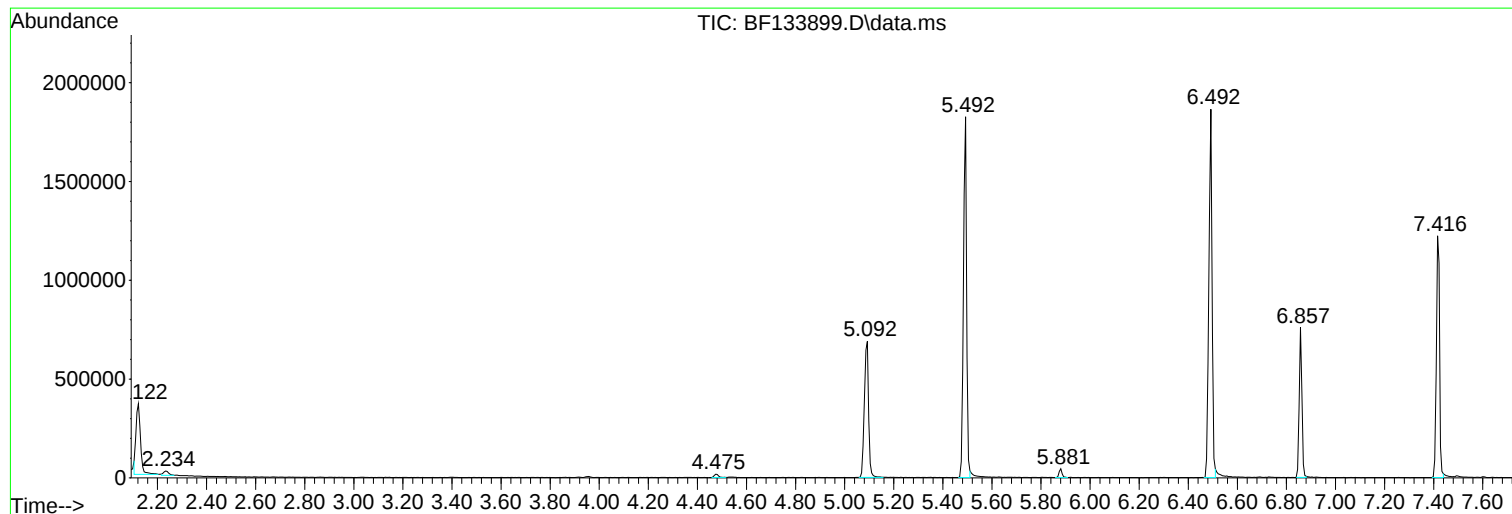
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ClientSampleId :
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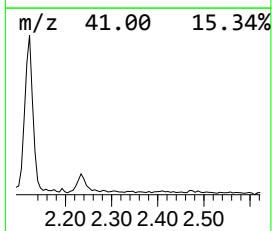
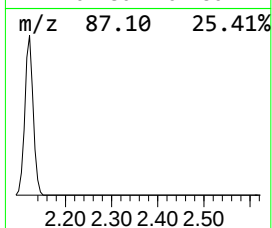
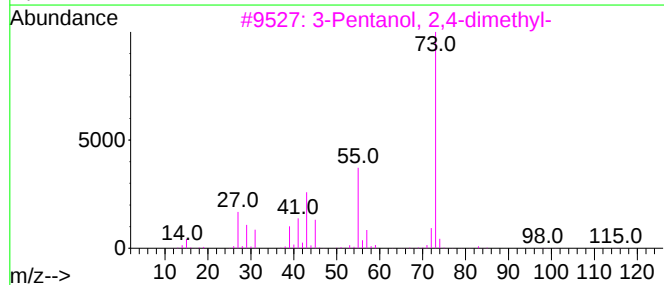
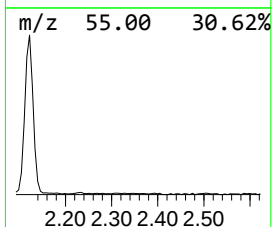
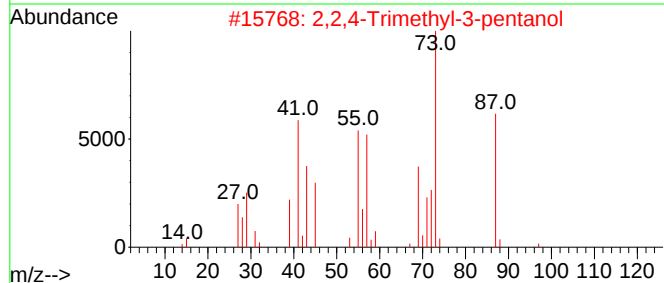
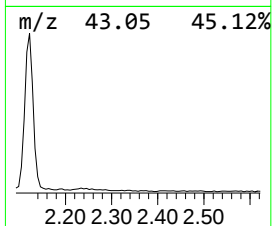
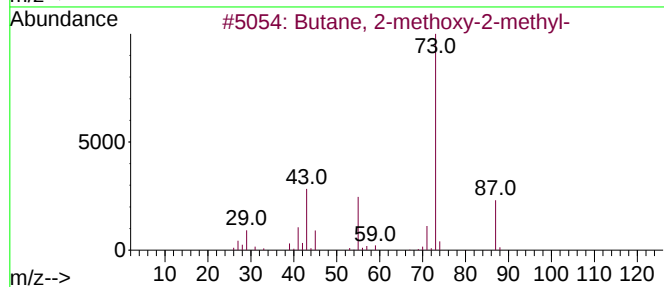
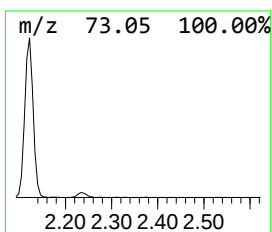
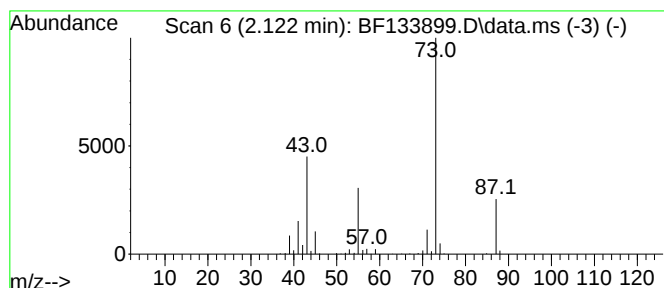
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	15.68 ng	457336	1,4-Dichlorobenzene-d4	6.857

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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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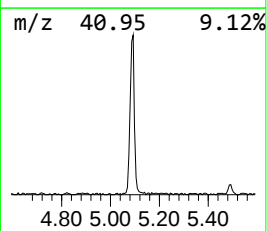
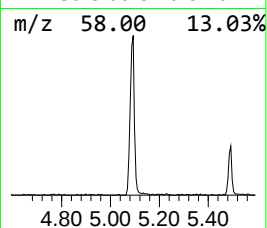
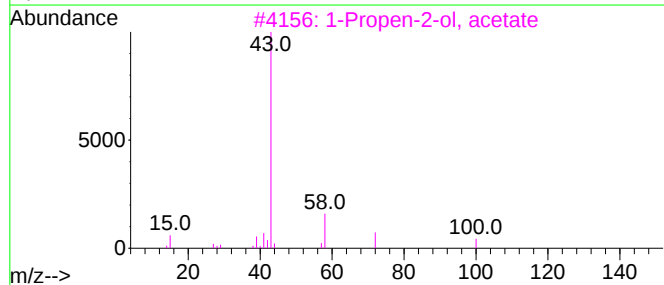
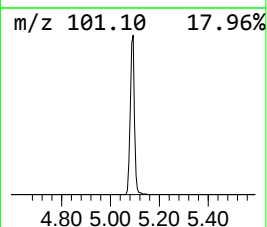
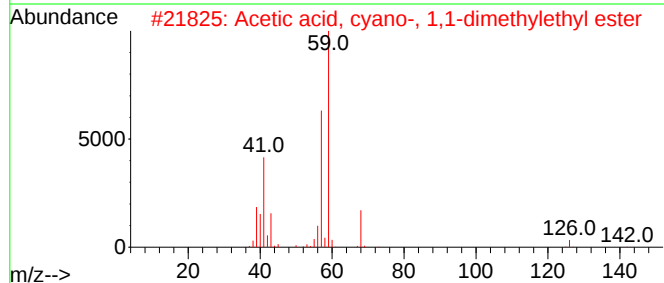
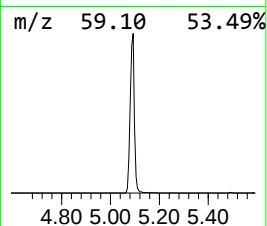
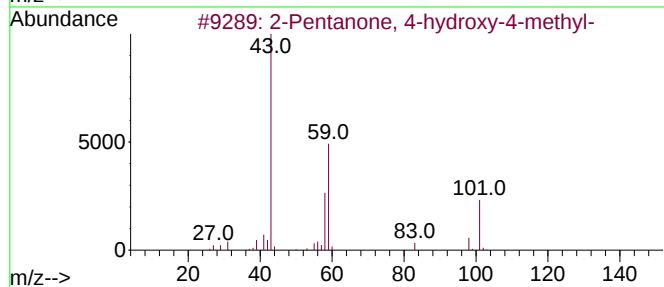
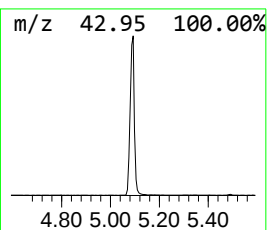
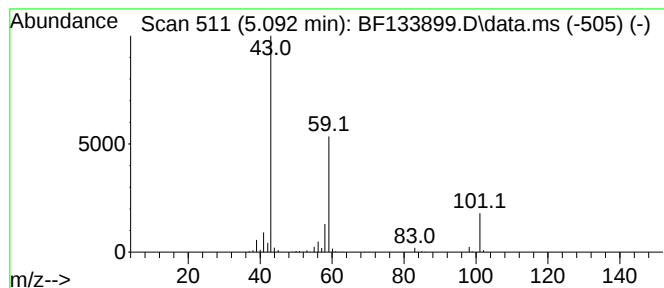
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	28.24 ng	823688	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9		



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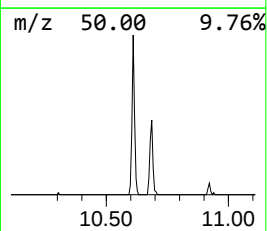
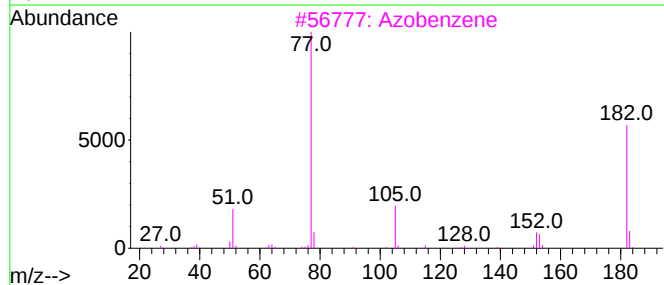
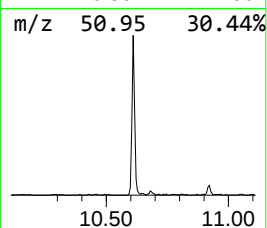
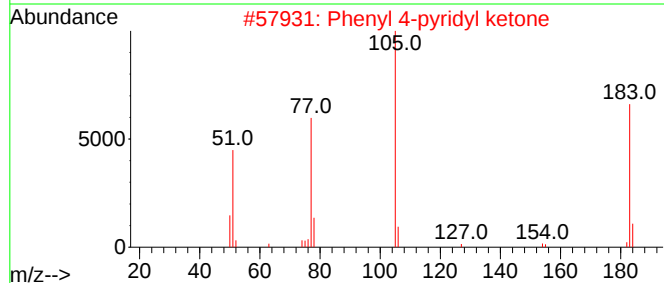
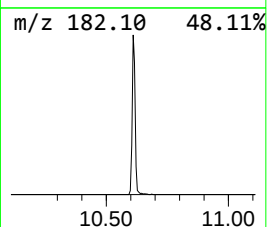
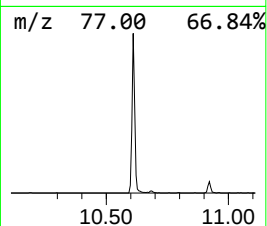
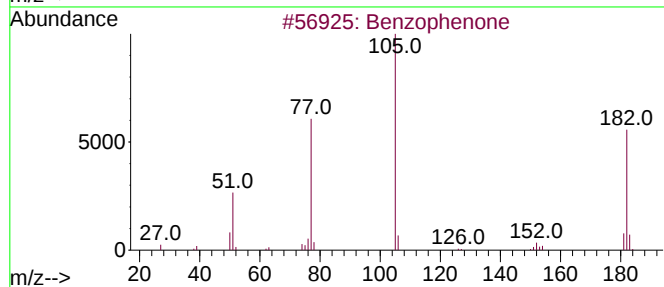
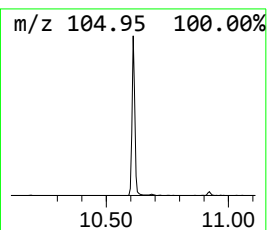
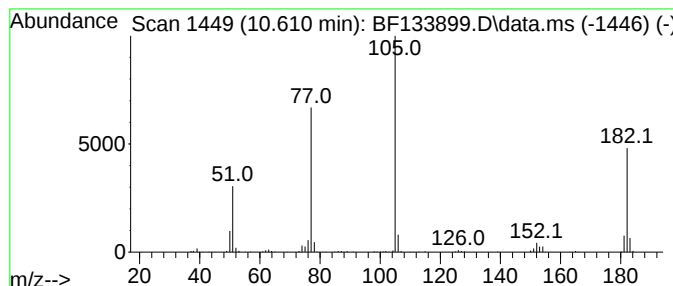
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	8.77 ng	338294	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			Azobenzene	182	C12H10N2	000103-33-3	53
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
5			.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	50



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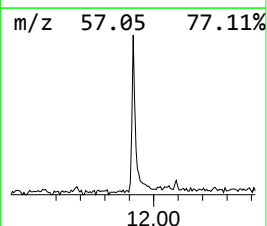
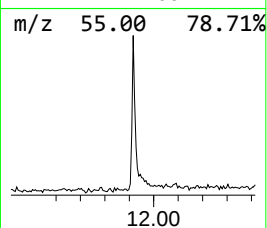
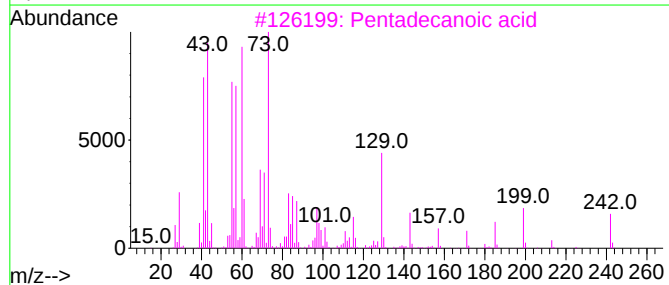
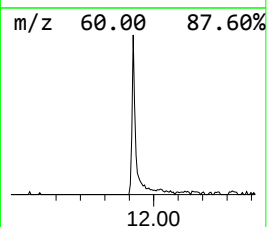
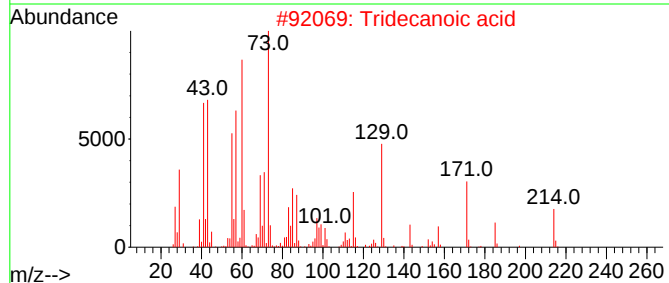
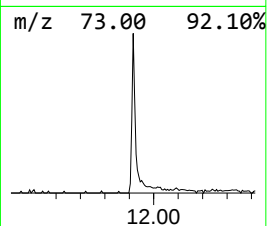
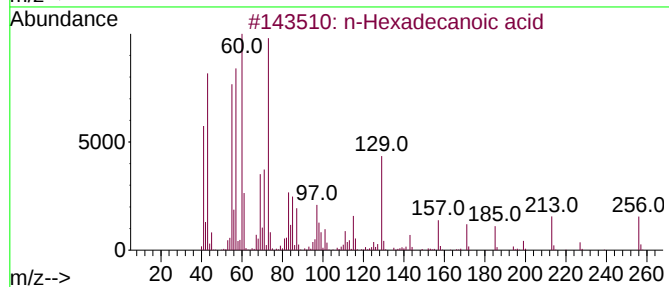
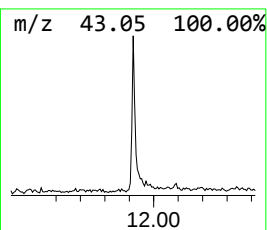
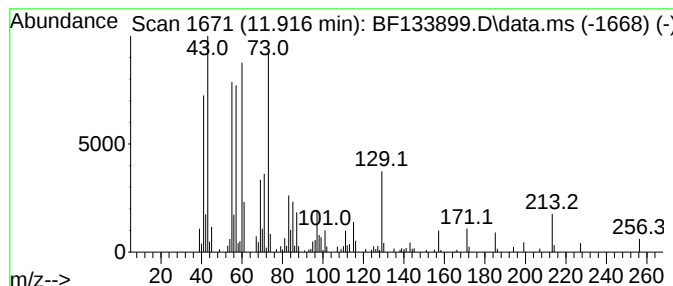
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	5.17 ng	183646	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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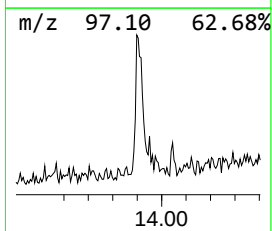
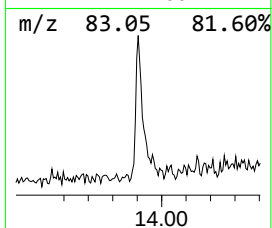
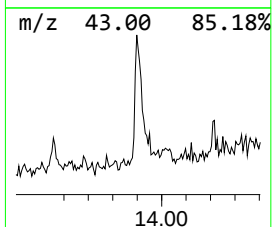
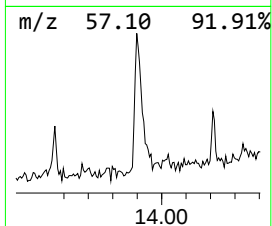
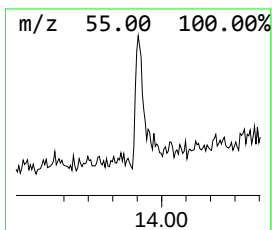
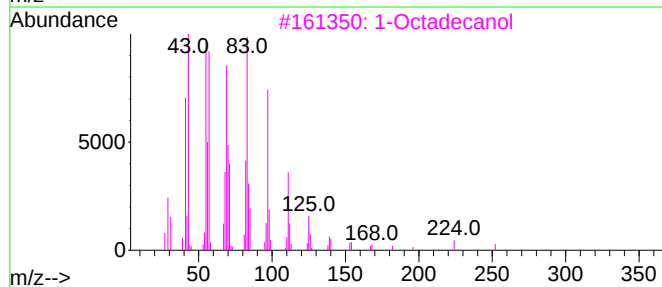
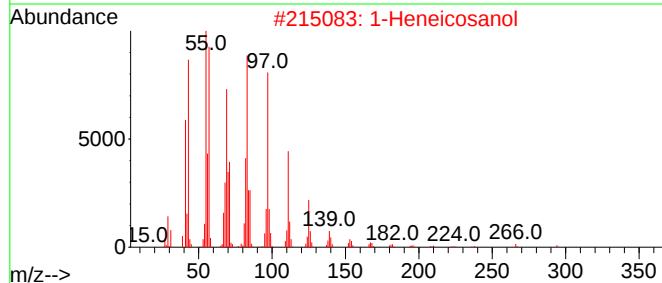
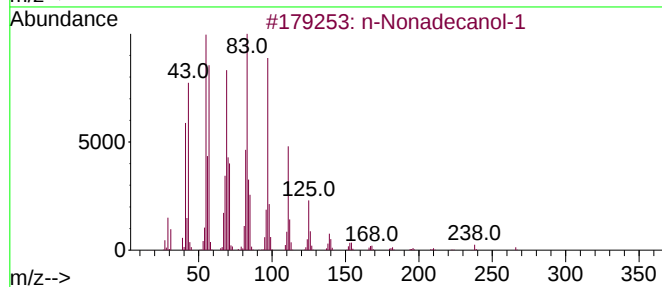
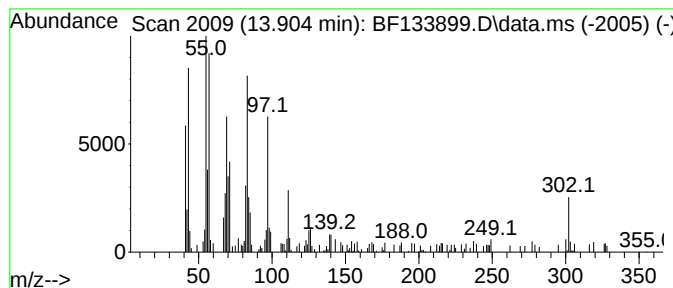
Instrument :
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Peak Number 5 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.904	4.85 ng	147239	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	81
2	1-Heneicosanol	312	C21H44O	015594-90-8	76
3	1-Octadecanol	270	C18H38O	000112-92-5	74
4	Behenic alcohol	326	C22H46O	000661-19-8	74
5	1-Tetracosene	336	C24H48	010192-32-2	70



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.122	15.7	ng	457336	1	6.857	583436	20.0
2-Pentanone, 4-...	5.092	28.2	ng	823688	1	6.857	583436	20.0
Benzophenone	10.610	8.8	ng	338294	3	9.892	771764	20.0
n-Hexadecanoic ...	11.916	5.2	ng	183646	4	11.386	710408	20.0
n-Nonadecanol-1	13.904	4.8	ng	147239	5	14.045	607251	20.0