

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031423\
 Data File : BF132783.D
 Acq On : 14 Mar 2023 17:49
 Operator : CG\JU
 Sample : 01891-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C0AA6

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: BF132783.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.593	338	341	349	rBV	134521	160632	2.38%	0.447%
2	5.193	439	443	454	rBV	1068759	1132625	16.81%	3.150%
3	5.593	508	511	530	rBV	2431870	2304357	34.20%	6.408%
4	5.981	573	577	584	rBV	219518	190767	2.83%	0.530%
5	6.593	677	681	698	rVB	1421228	1380413	20.49%	3.839%
6	6.963	740	744	748	rBV	1600791	1269956	18.85%	3.532%
7	7.534	836	841	844	rBV	3722465	3766462	55.90%	10.474%
8	8.245	959	962	966	rBV	1955876	1639993	24.34%	4.561%
9	9.328	1141	1146	1149	rBV	6239536	6249665	92.76%	17.379%
10	10.004	1258	1261	1265	rBV	2204365	1890812	28.06%	5.258%
11	10.722	1379	1383	1386	rBV	346953	280479	4.16%	0.780%
12	10.804	1392	1397	1400	rBV	4278277	4160995	61.76%	11.571%
13	11.498	1512	1515	1519	rBV	2199533	2009341	29.82%	5.588%
14	12.010	1599	1602	1608	rBV	64866	79248	1.18%	0.220%
15	13.092	1781	1786	1789	rBV	6780884	6737798	100.00%	18.737%
16	13.969	1931	1935	1951	rBV	145865	240547	3.57%	0.669%
17	14.157	1962	1967	1976	rVB	1167186	1182155	17.55%	3.287%
18	14.998	2106	2110	2116	rBV2	77523	82369	1.22%	0.229%
19	15.686	2221	2227	2233	rBV	930426	1201580	17.83%	3.341%

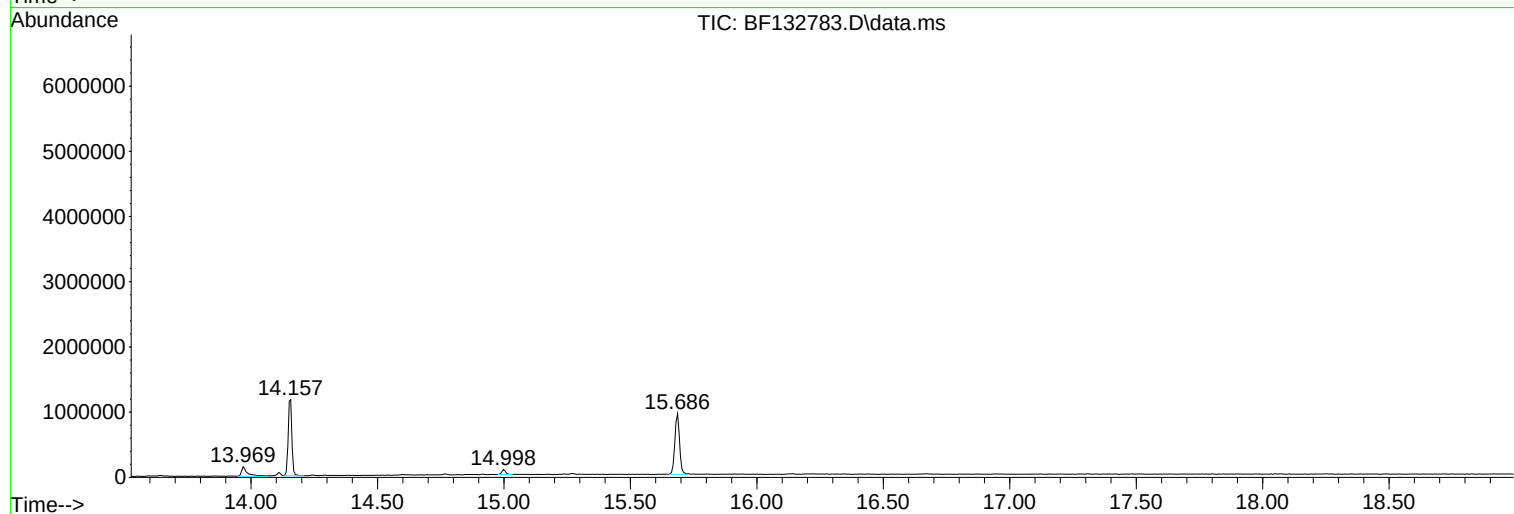
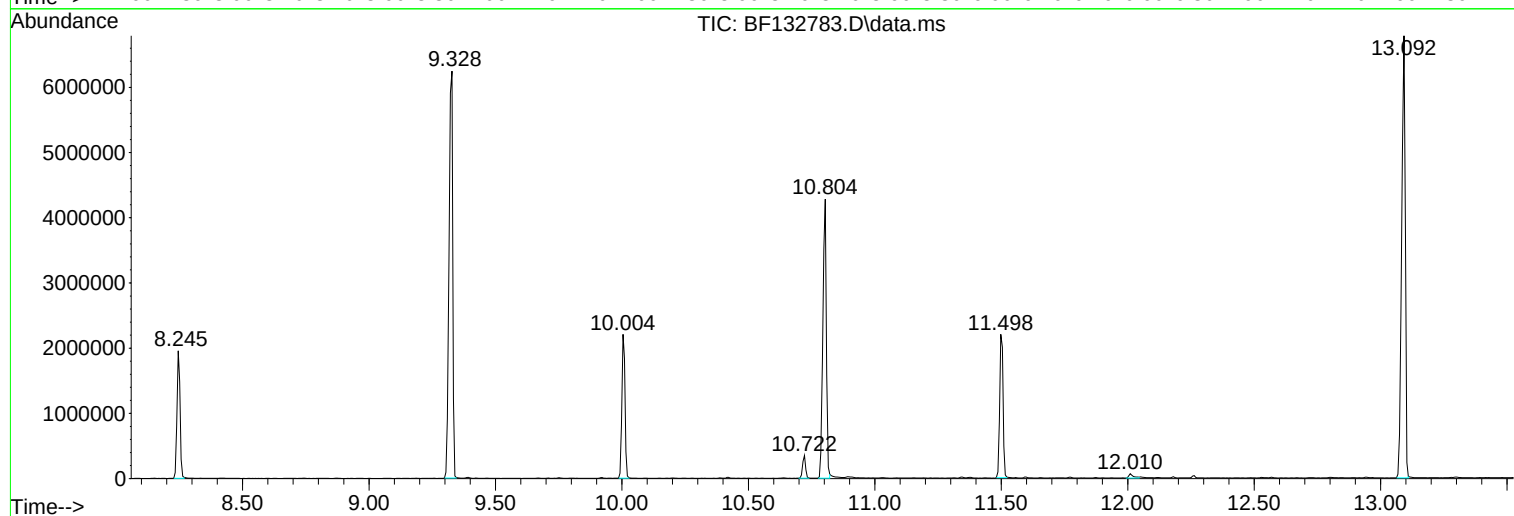
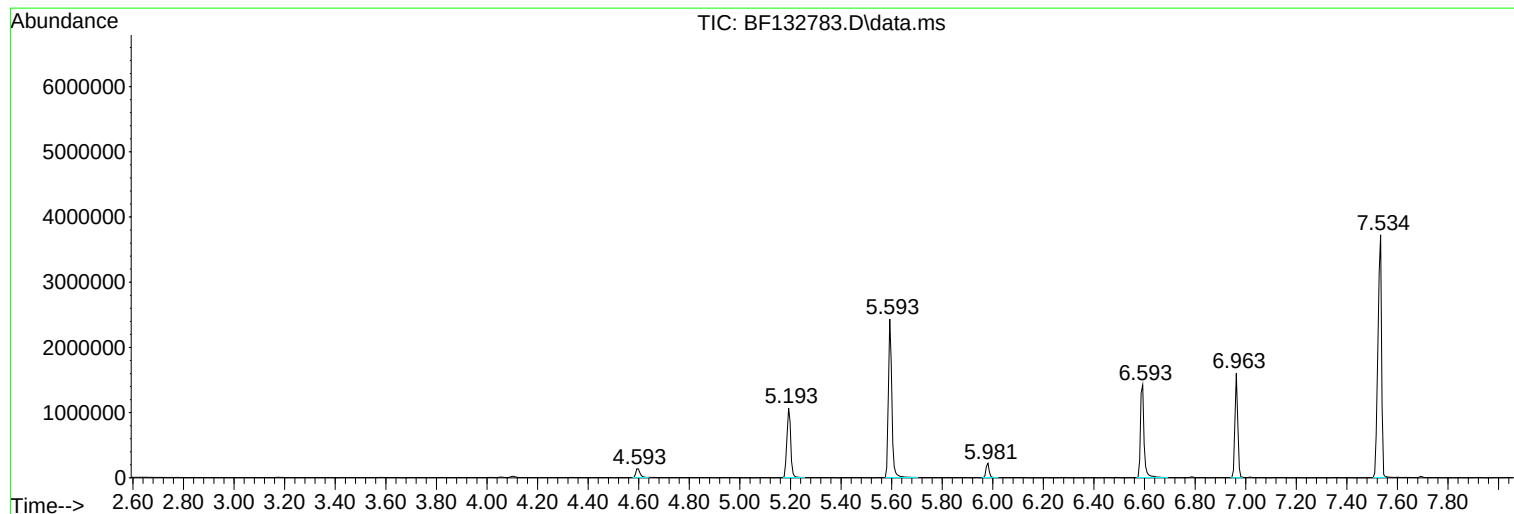
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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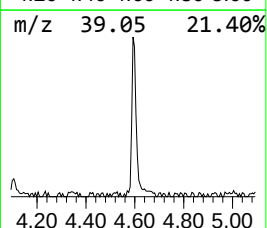
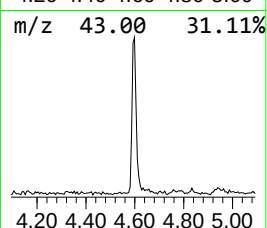
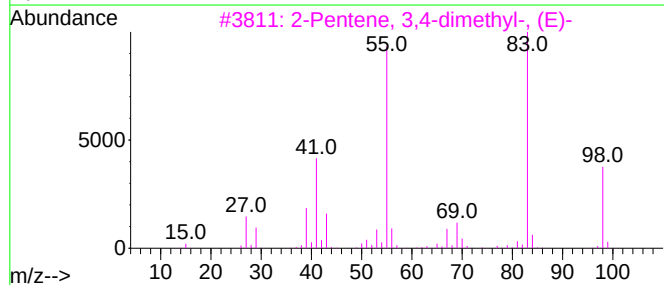
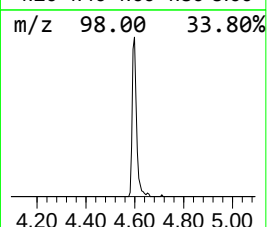
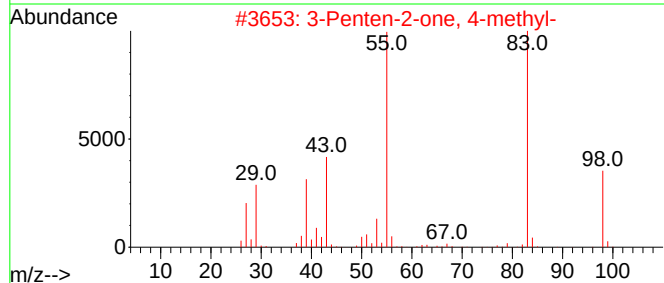
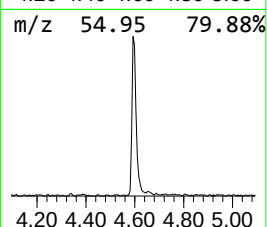
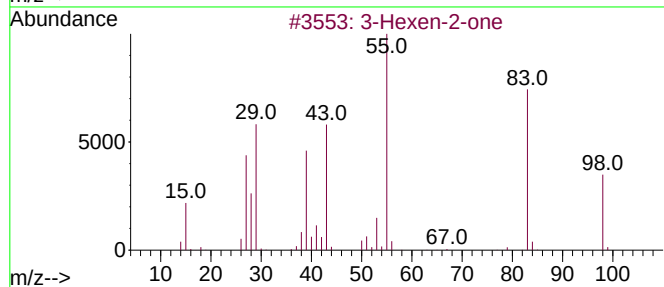
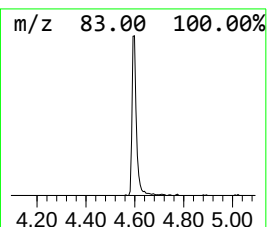
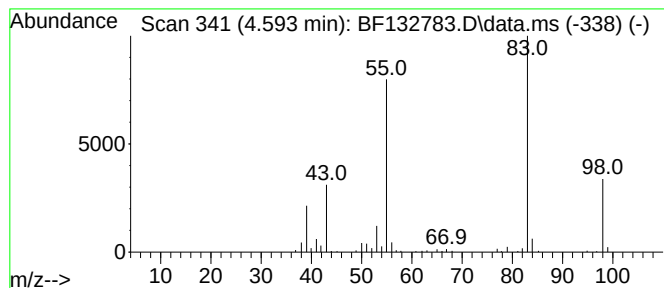
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.593	2.53 ng	160632	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	86
4			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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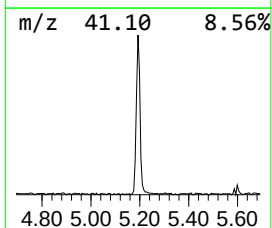
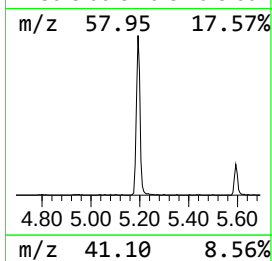
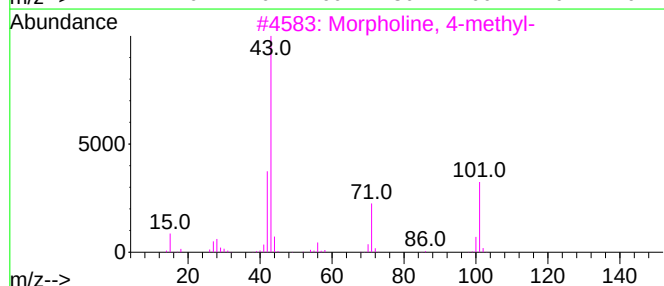
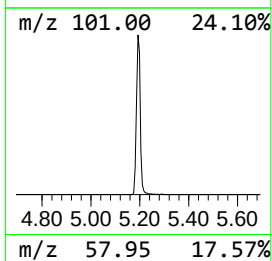
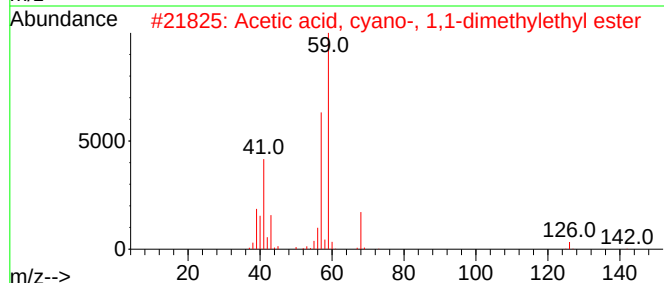
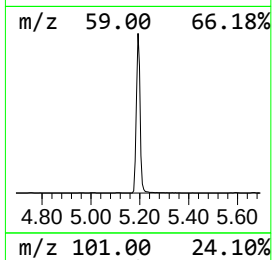
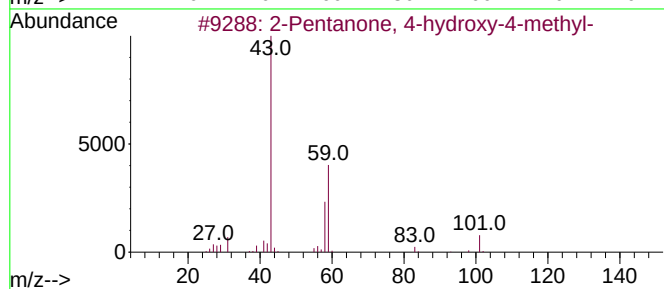
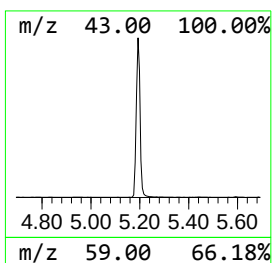
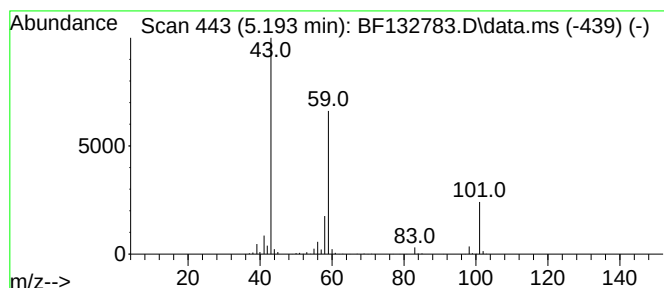
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.193	17.84 ng	1132630	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			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Acetone	58	C3H6O	000067-64-1	9
5			Guanidine	59	CH5N3	000113-00-8	9



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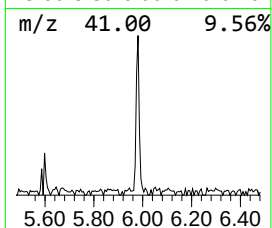
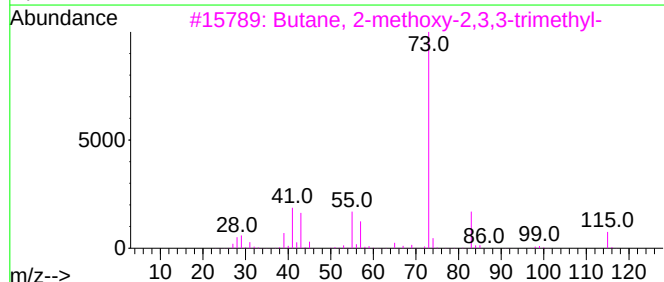
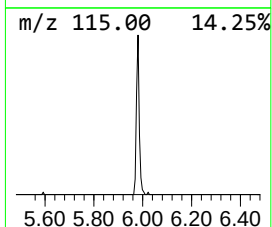
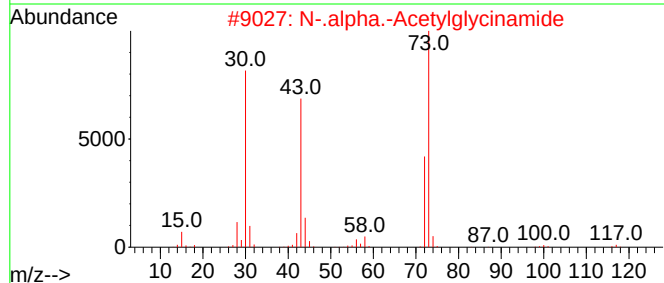
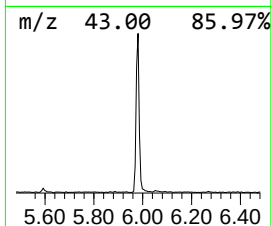
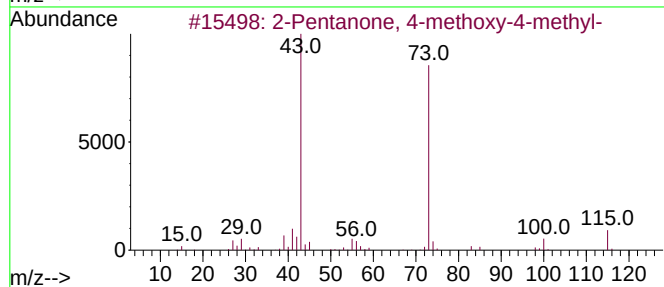
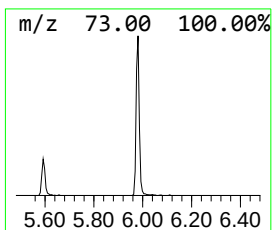
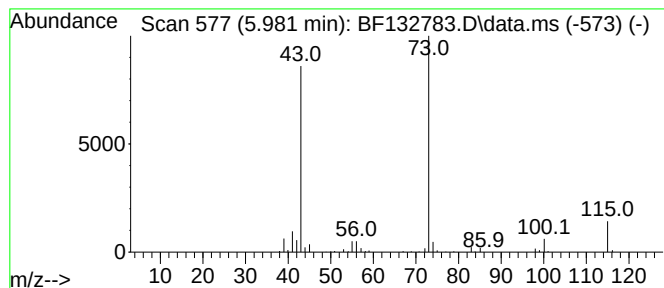
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.981	3.00 ng	190767	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	59
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	25
3			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
4			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12



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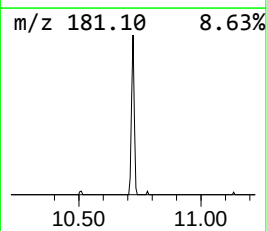
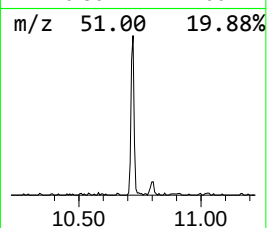
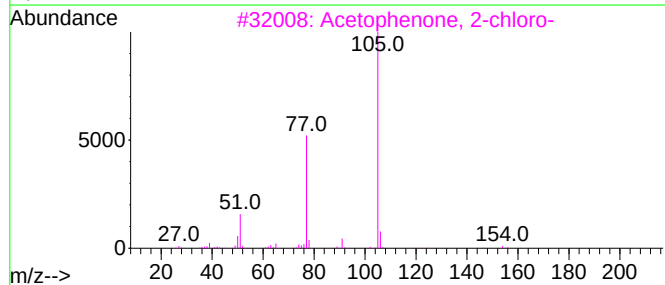
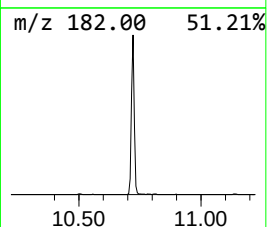
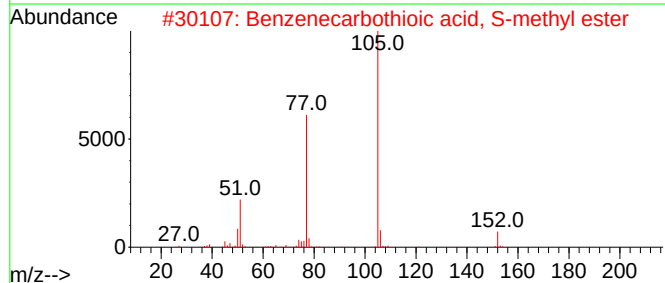
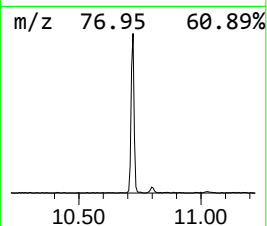
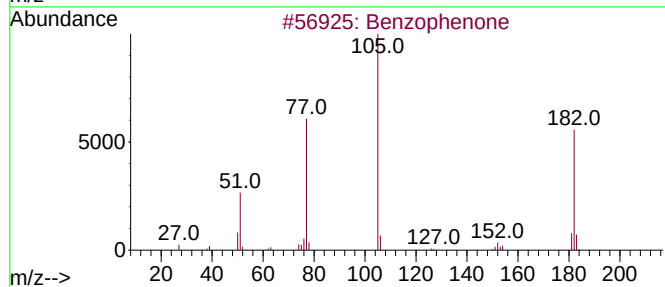
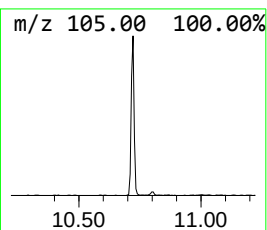
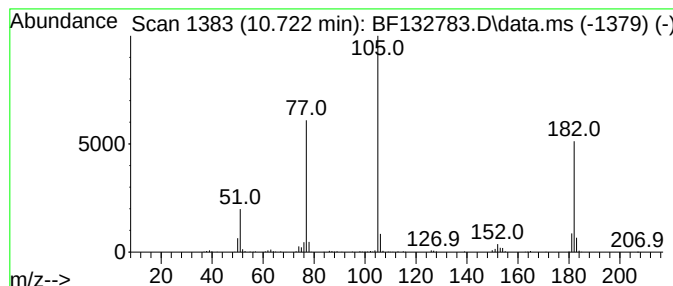
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.722	2.97 ng	280479	Acenaphthene-d10	10.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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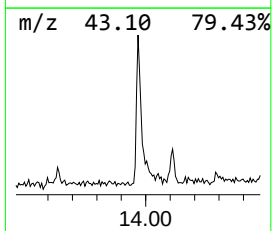
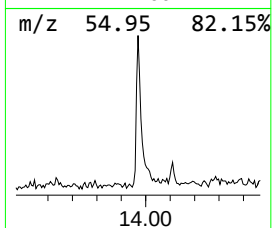
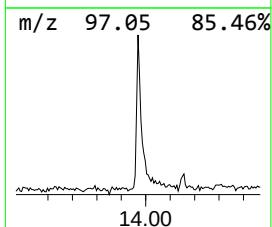
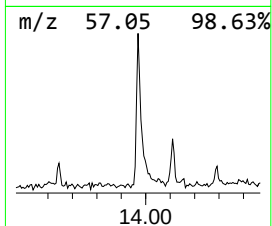
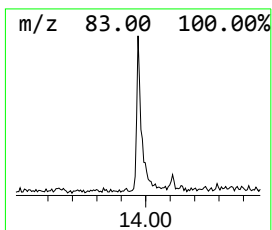
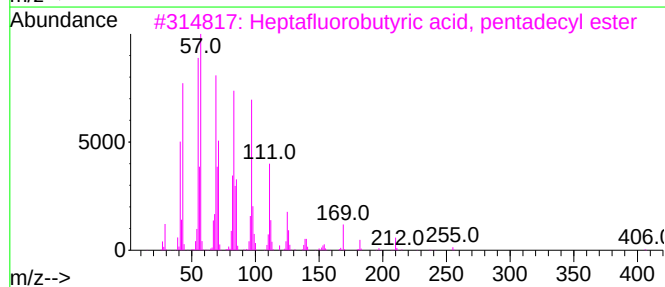
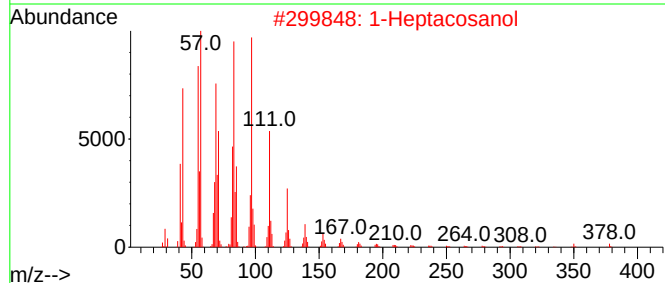
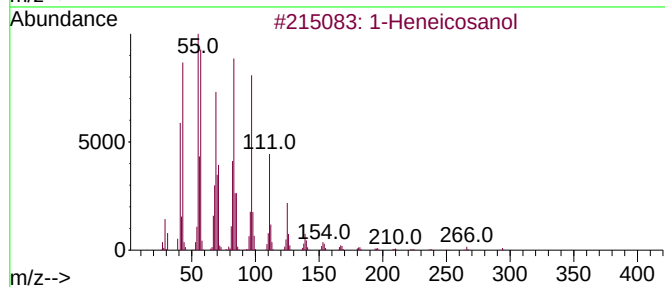
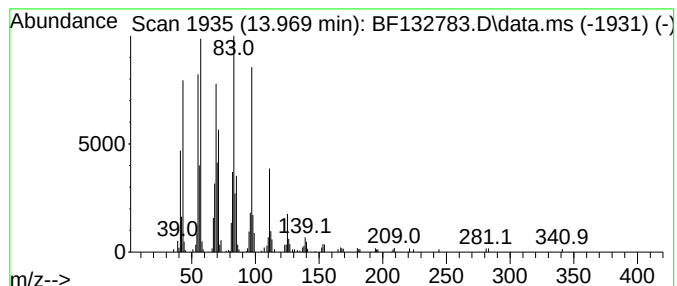
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	4.07 ng	240547	Chrysene-d12	14.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Heptacosanol	396	C27H56O	002004-39-9	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4			1-Hexacosanol	382	C26H54O	000506-52-5	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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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
3-Hexen-2-one	4.593	2.5	ng	160632	1	6.963	1269960	20.0
2-Pentanone, 4-...	5.193	17.8	ng	1132630	1	6.963	1269960	20.0
2-Pentanone, 4-...	5.981	3.0	ng	190767	1	6.963	1269960	20.0
Benzophenone	10.722	3.0	ng	280479	3	10.004	1890810	20.0
1-Heneicosanol	13.969	4.1	ng	240547	5	14.157	1182160	20.0