

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100522\
 Data File : BM036833.D
 Acq On : 05 Oct 2022 11:05
 Operator : CG/JU
 Sample : PB147982BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB147982BL

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_M\Methods\8270-BM100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036833.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.834	122	127	139	rVB	648538	759963	4.04%	0.713%
2	4.452	227	232	248	rBV	3525455	4425640	23.53%	4.153%
3	4.575	248	253	260	rBV	147023	211697	1.13%	0.199%
4	5.069	330	337	350	rBV	3522591	4814389	25.60%	4.517%
5	5.534	409	416	439	rVB	8395746	11982293	63.71%	11.243%
6	6.152	516	521	531	rVB	149991	223354	1.19%	0.210%
7	7.140	676	689	710	rBV	7822961	12858271	68.36%	12.065%
8	7.975	823	831	840	rBV	1348661	2103644	11.18%	1.974%
9	9.140	1020	1029	1042	rBV	4581535	7414636	39.42%	6.957%
10	10.781	1299	1308	1321	rBV	1836862	3001415	15.96%	2.816%
11	13.233	1717	1725	1737	rBV	11454190	16512752	87.79%	15.494%
12	14.598	1950	1957	1967	rBV	2498058	3667687	19.50%	3.441%
13	16.080	2202	2209	2236	rBV	7804887	10999738	58.48%	10.321%
14	17.333	2416	2422	2432	rBV	2797115	4011126	21.33%	3.764%
15	19.951	2861	2867	2882	rBV	15876530	18808306	100.00%	17.648%
16	21.503	3126	3131	3140	rBV	2397490	3021329	16.06%	2.835%
17	23.915	3536	3541	3557	rVB2	822354	1756303	9.34%	1.648%

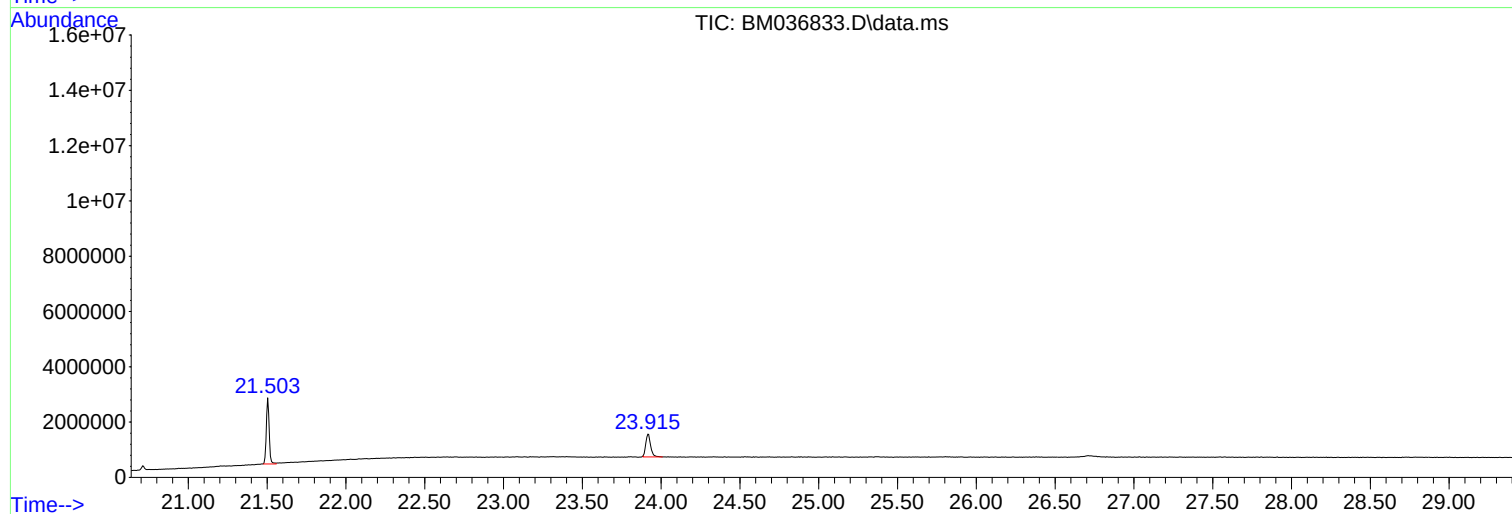
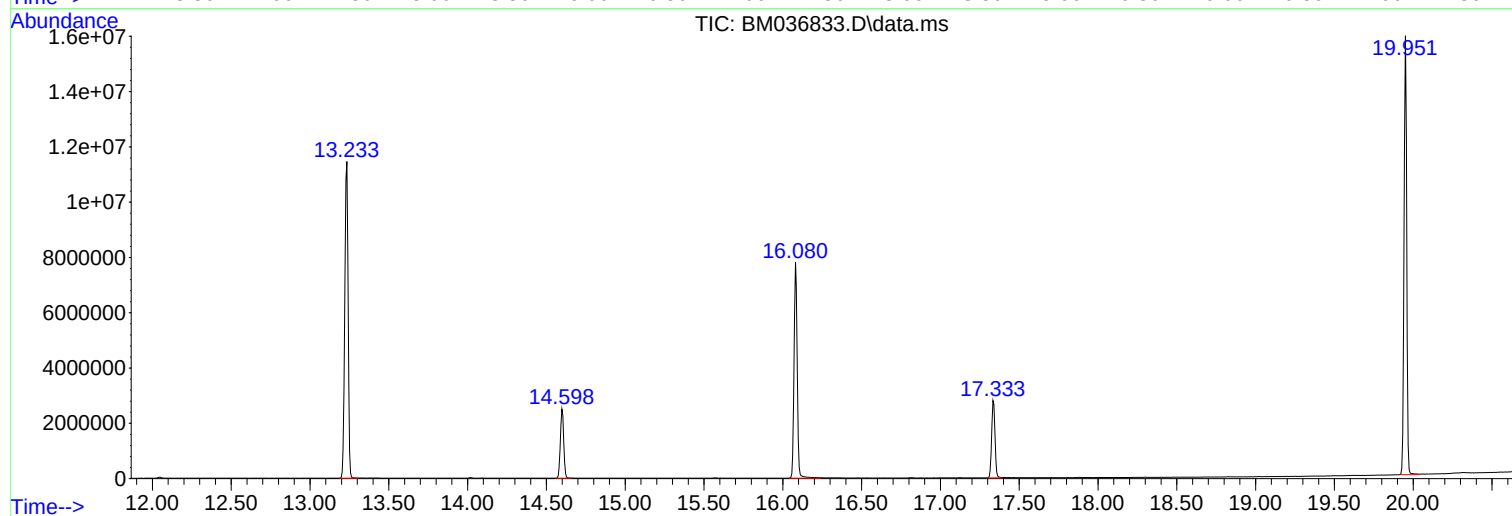
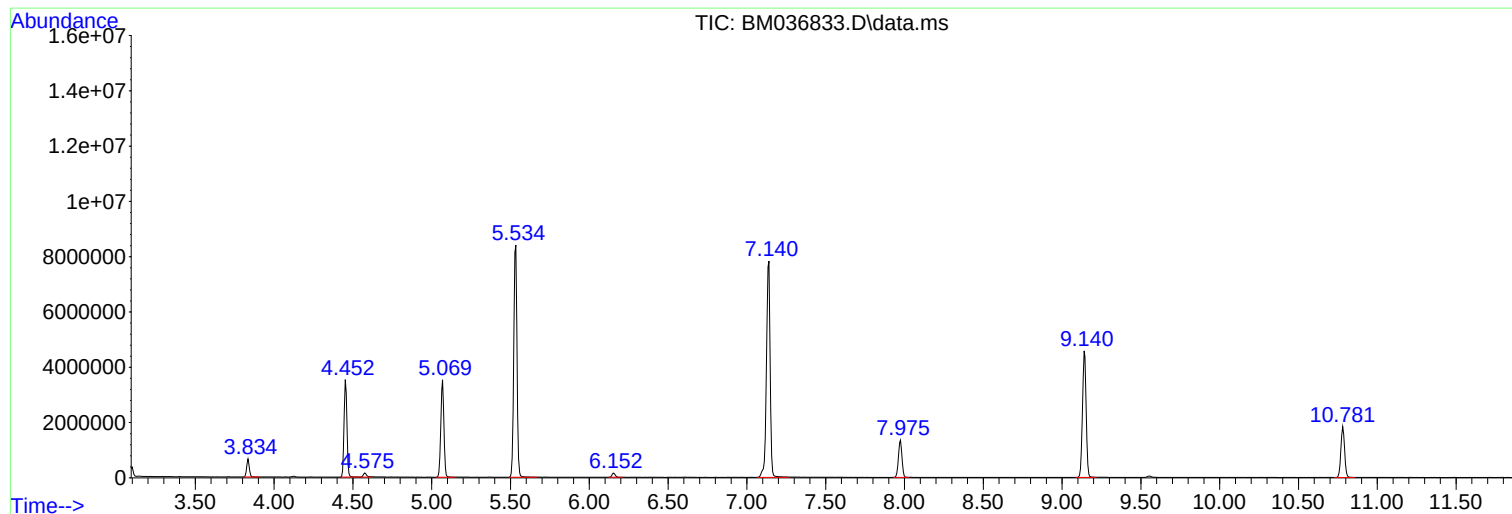
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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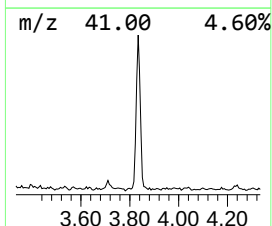
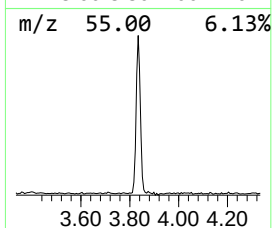
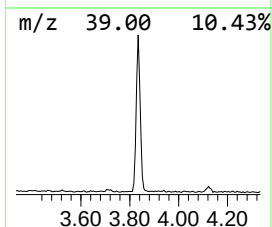
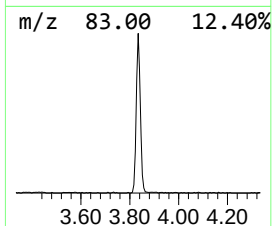
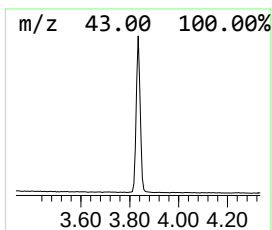
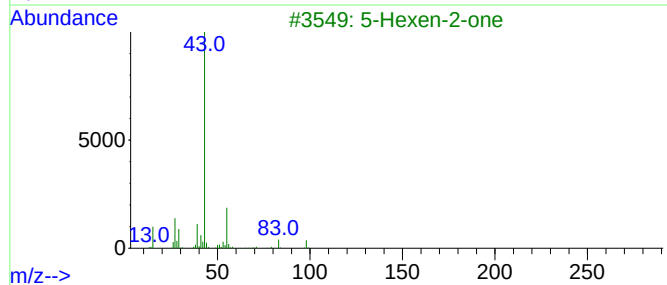
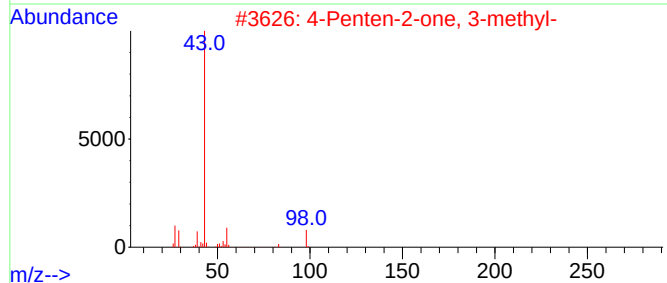
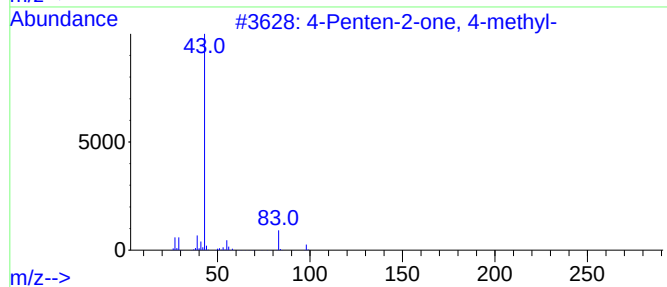
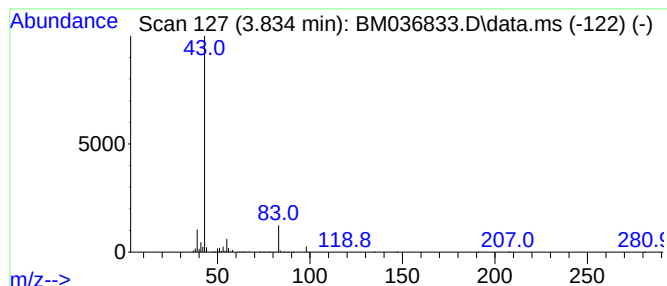
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.834	7.23 ng	759963	1,4-Dichlorobenzene-d4	7.975

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	50
3		5-Hexen-2-one	98	C6H10O	000109-49-9	50
4		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	30
5		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	23



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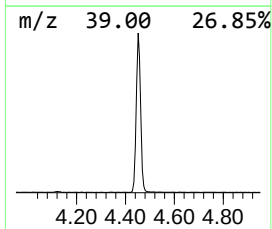
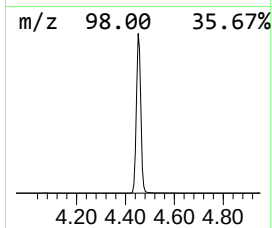
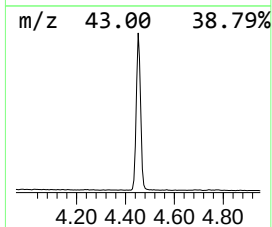
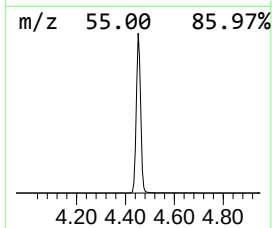
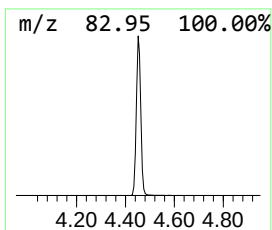
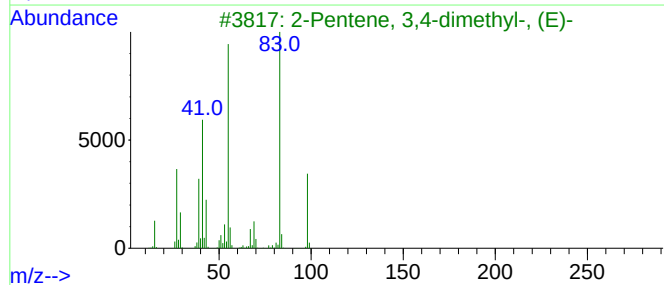
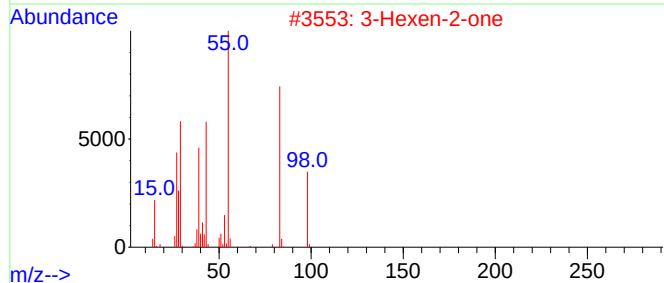
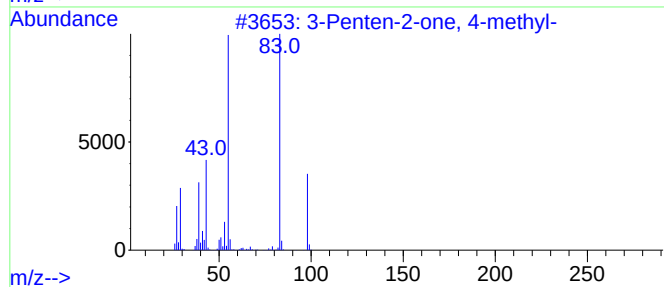
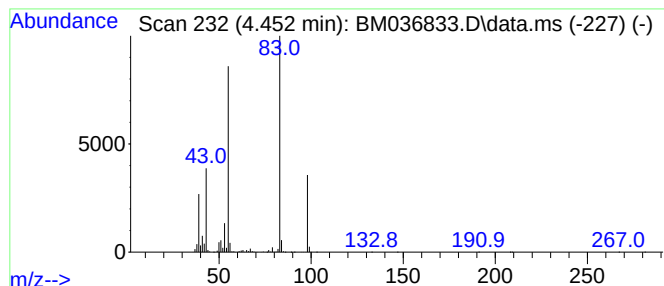
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.452	42.08 ng	4425640	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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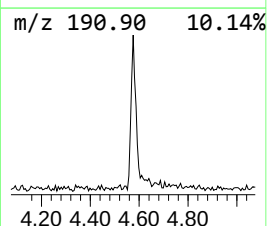
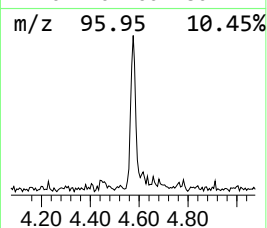
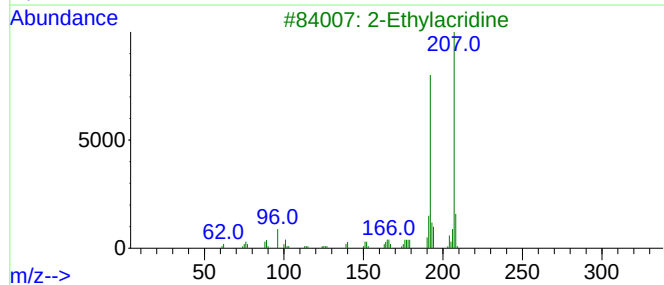
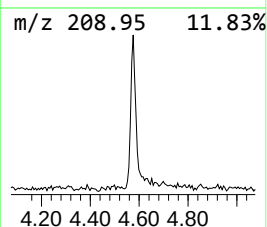
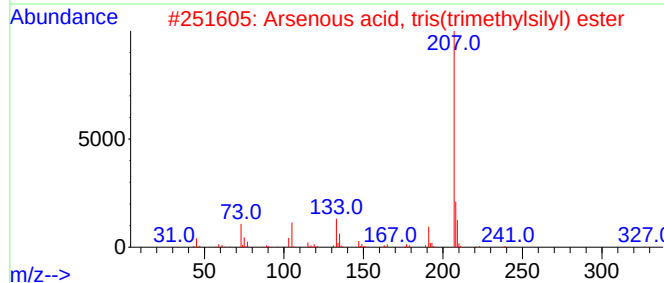
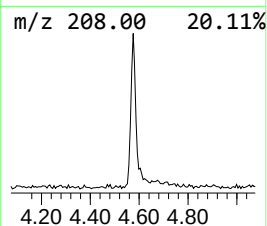
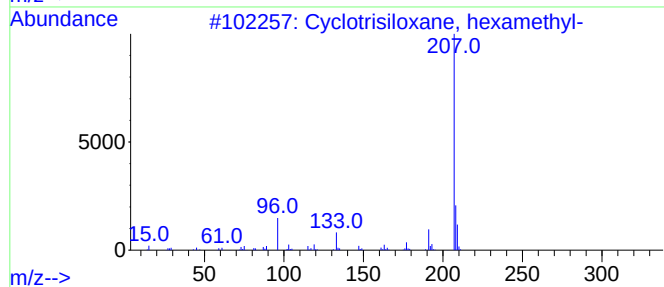
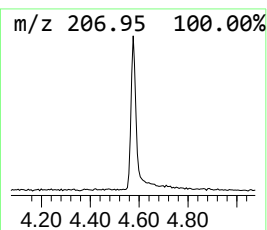
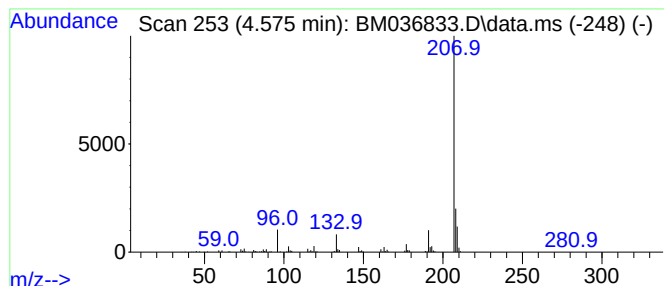
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Cyclotrisiloxane, hexamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.575	2.01 ng	211697	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	91
2			Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	72
3			2-Ethylacridine	207	C15H13N	055751-83-2	45
4			Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	39
5			4-tert-Octylphenol, TMS derivative	278	C17H30OSi	078721-87-6	39



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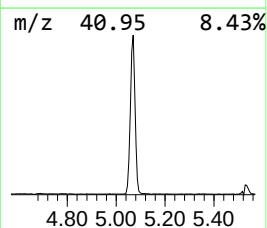
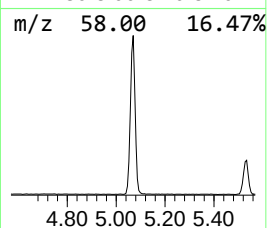
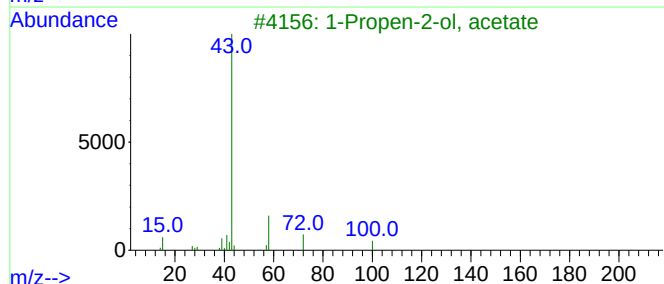
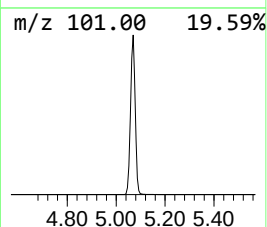
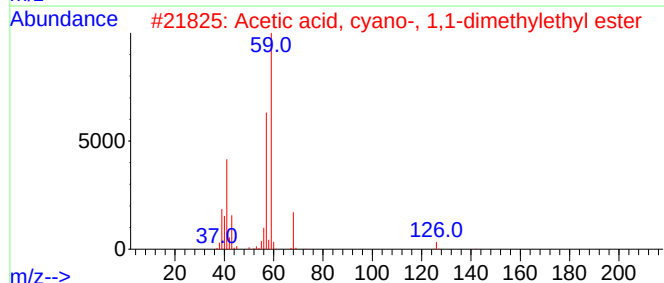
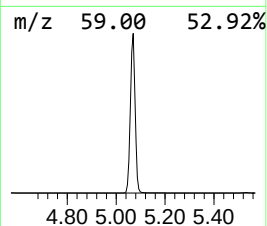
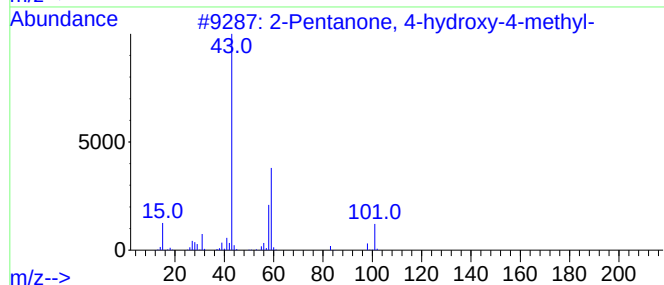
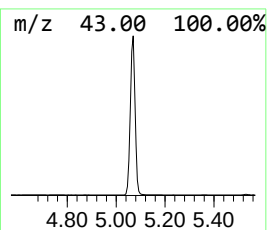
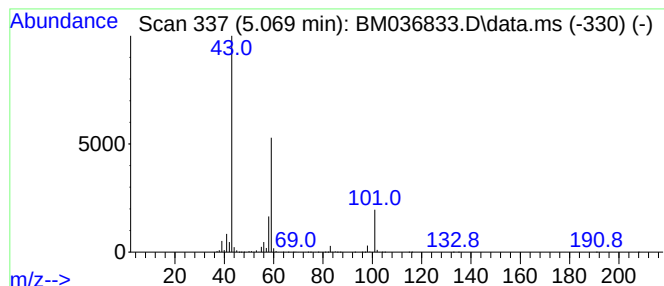
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.069	45.77 ng	4814390	1,4-Dichlorobenzene-d4	7.975	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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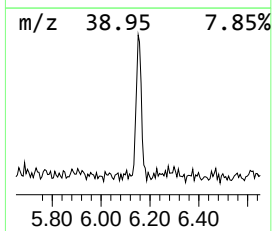
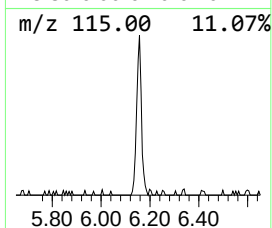
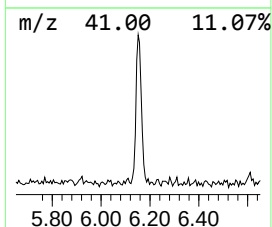
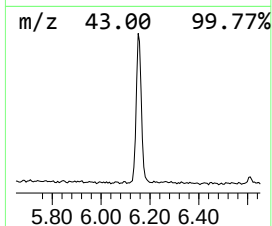
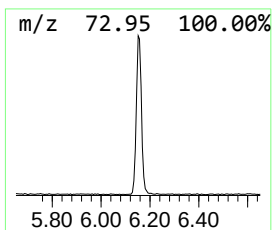
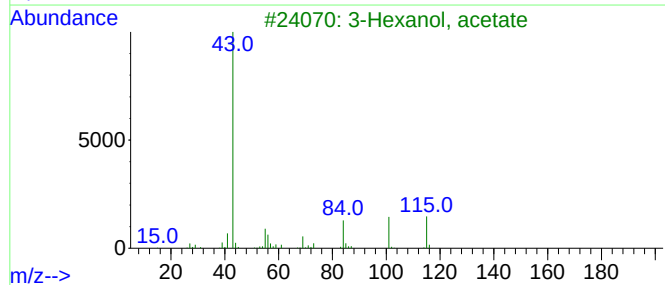
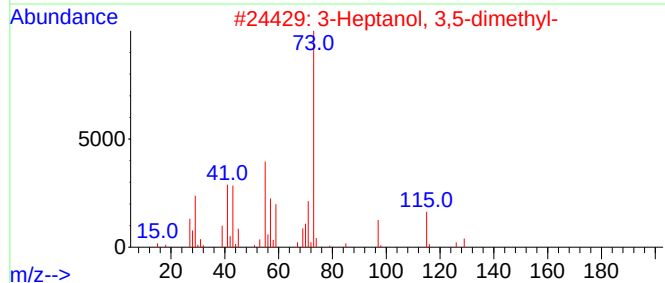
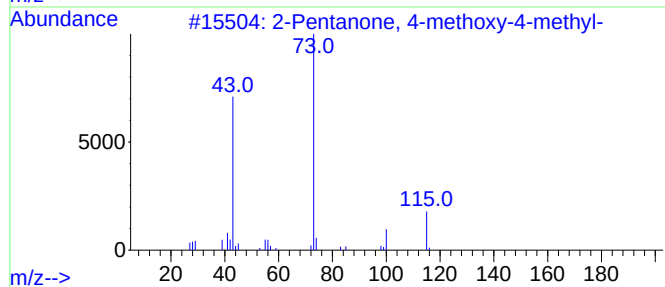
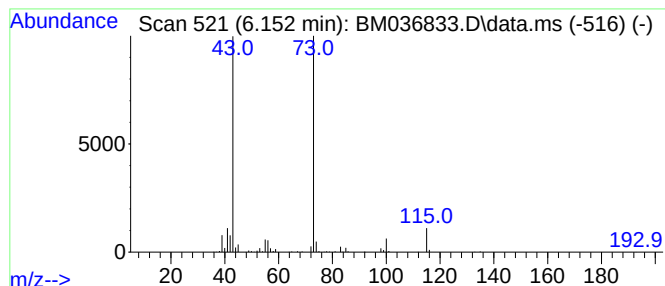
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Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.152	2.12 ng	223354	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	25
3			3-Hexanol, acetate	144	C8H16O2	040780-64-1	25
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	25
5			N-Ethylformamide	73	C3H7NO	000627-45-2	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one,...	3.834	7.2	ng	759963	1	7.975	2103640	20.0
3-Penten-2-one,...	4.452	42.1	ng	4425640	1	7.975	2103640	20.0
Cyclotrisiloxan...	4.575	2.0	ng	211697	1	7.975	2103640	20.0
2-Pentanone, 4-...	5.069	45.8	ng	4814390	1	7.975	2103640	20.0
2-Pentanone, 4-...	6.152	2.1	ng	223354	1	7.975	2103640	20.0