

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
 Data File : BF135621.D
 Acq On : 06 Oct 2023 10:51
 Operator : CG\JU
 Sample : PB156122BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB156122BL

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135621.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.463	227	234	250	rBV	693632	1194659	25.65%	3.270%
2	4.351	381	385	403	rBV	1902771	2439785	52.38%	6.678%
3	4.616	423	430	435	rVB	1688598	188858	4.05%	0.517%
4	4.981	487	492	508	rBV	1481953	2261555	48.55%	6.190%
5	5.387	557	561	584	rBV	3921064	4292476	92.15%	11.749%
6	5.763	621	625	636	rBV	98785	92582	1.99%	0.253%
7	6.357	723	726	728	rBV	143269	118698	2.55%	0.325%
8	6.392	728	732	758	rVB	3558633	4464848	95.85%	12.220%
9	6.739	787	791	803	rBV	938505	883979	18.98%	2.419%
10	7.304	882	887	900	rBV	2547351	2962842	63.61%	8.109%
11	8.016	1003	1008	1020	rBV	1215102	1162185	24.95%	3.181%
12	9.098	1186	1192	1195	rBV	4462625	4658017	100.00%	12.749%
13	9.775	1302	1307	1311	rBV	1445822	1277237	27.42%	3.496%
14	10.574	1438	1443	1459	rBV	2876349	3045606	65.38%	8.336%
15	11.269	1557	1561	1570	rBV	1632364	1379355	29.61%	3.775%
16	12.868	1828	1833	1836	rBV	4148499	4579860	98.32%	12.535%
17	13.927	2009	2013	2020	rBV	1048737	1068997	22.95%	2.926%
18	15.398	2259	2263	2274	rBV2	312310	464670	9.98%	1.272%

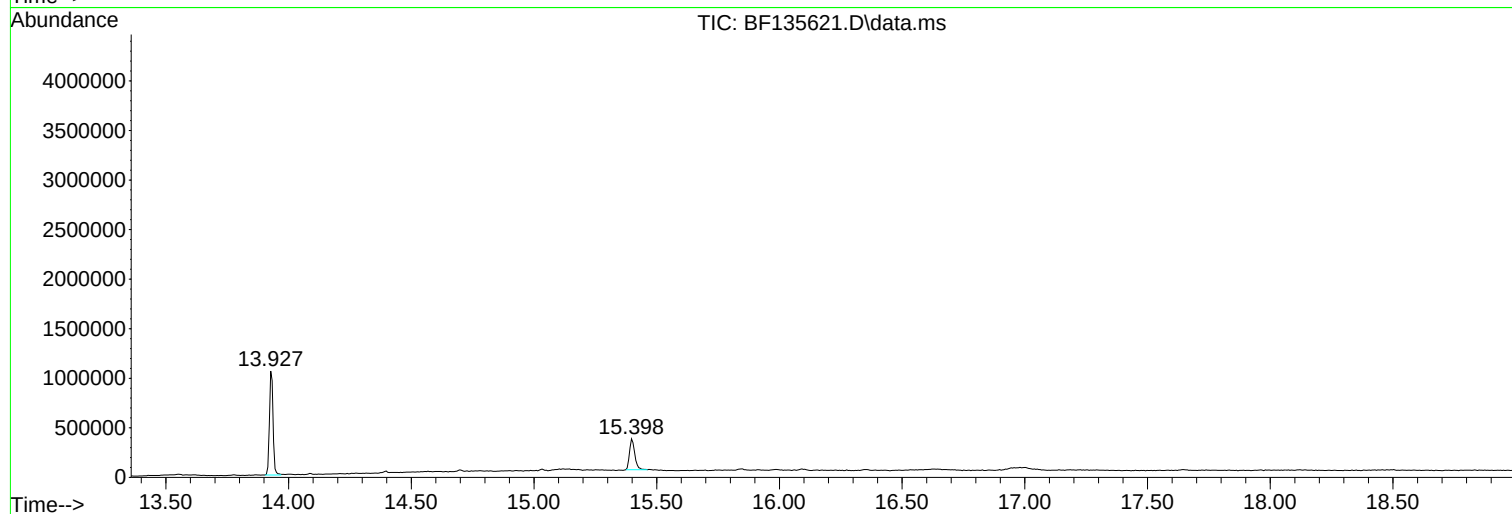
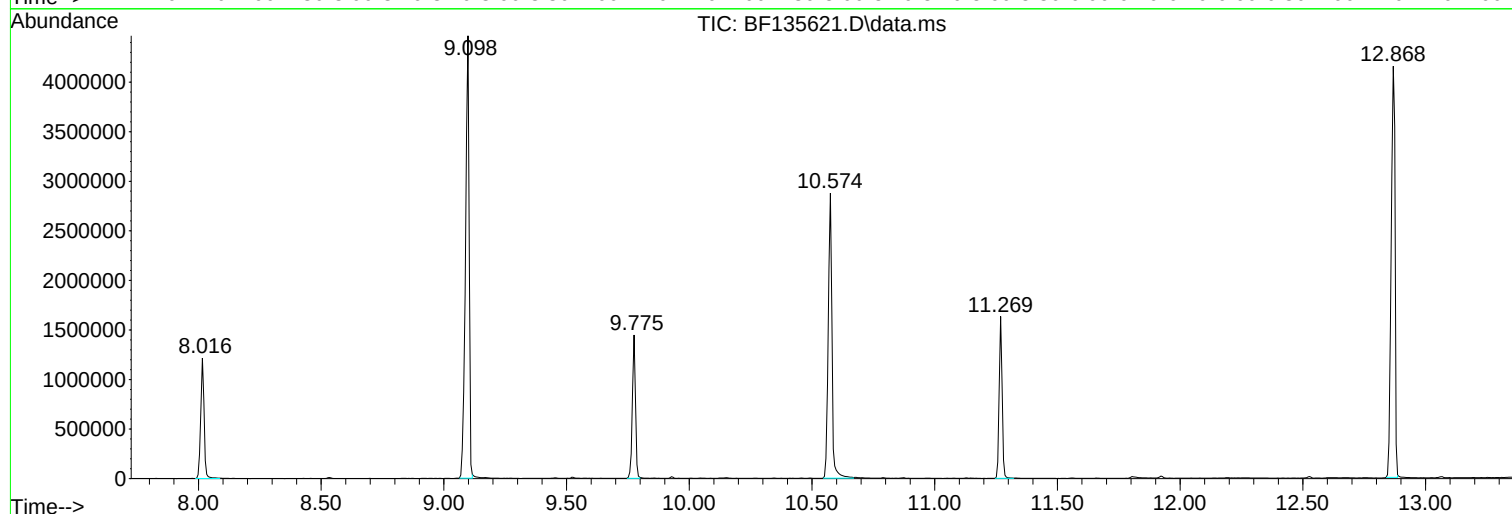
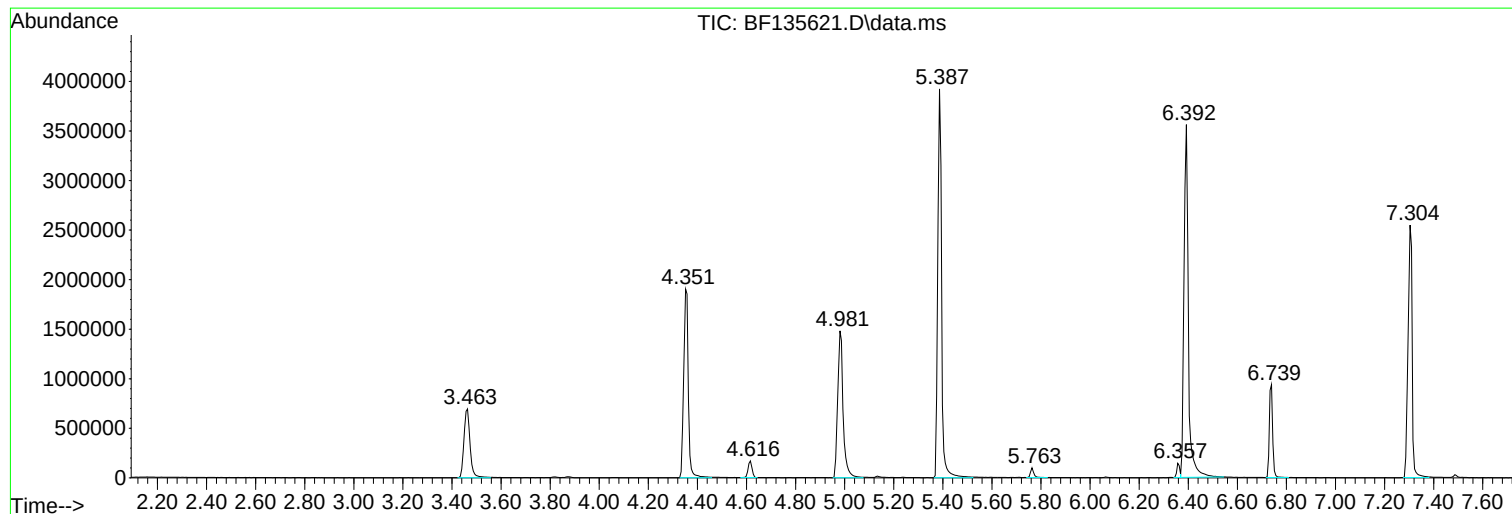
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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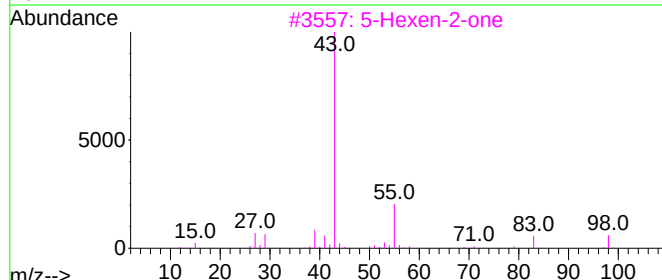
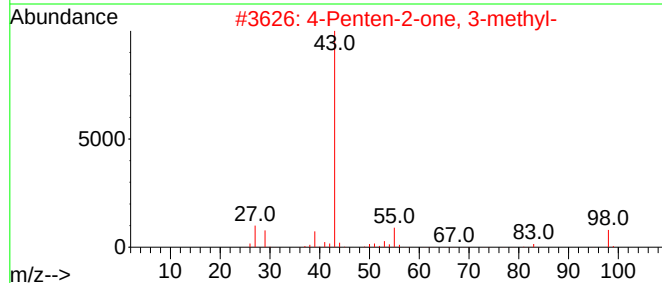
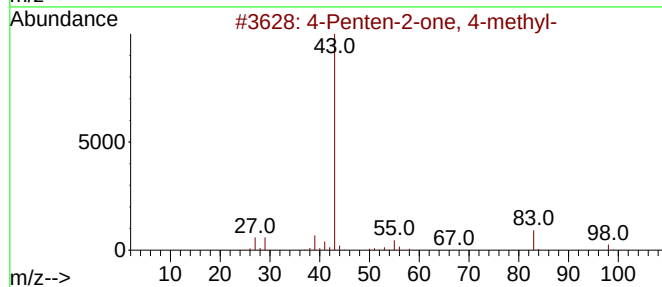
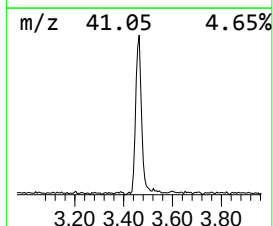
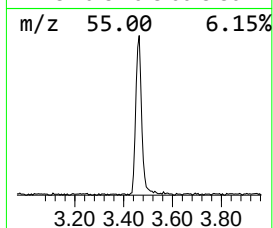
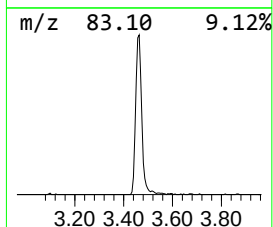
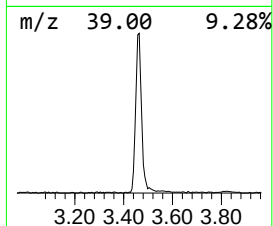
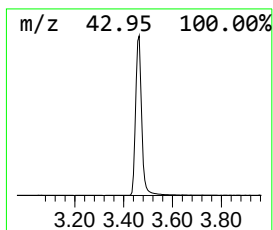
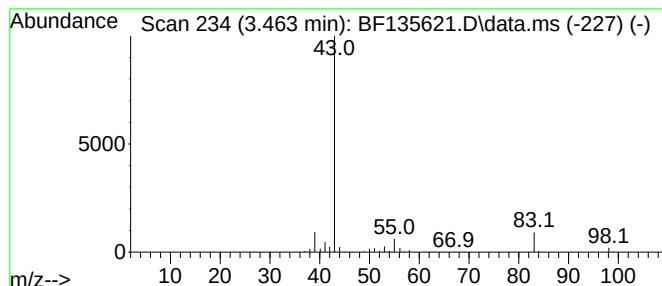
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.463	27.03 ng	1194660	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	50
3			5-Hexen-2-one	98	C6H10O	000109-49-9	38
4			Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	16
5			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9



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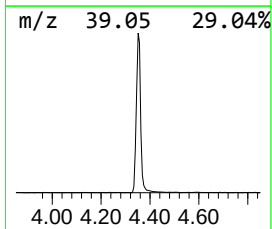
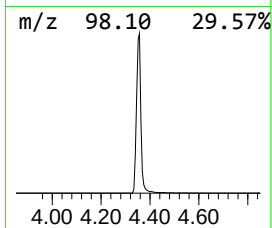
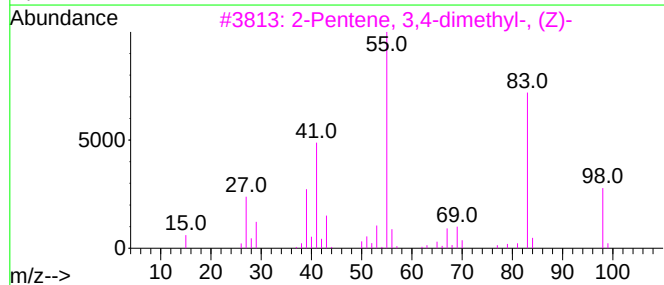
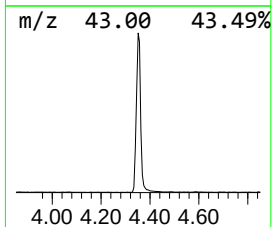
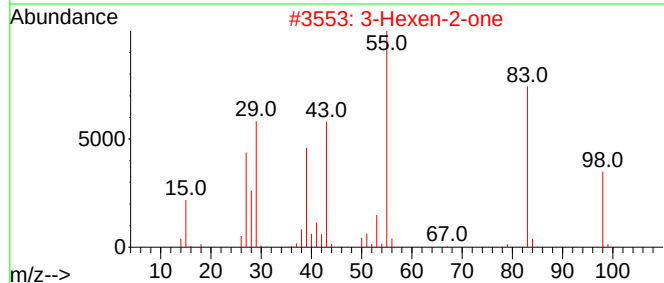
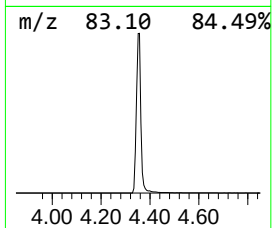
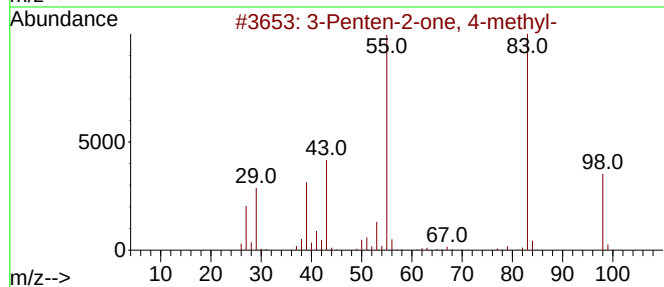
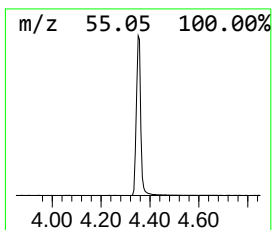
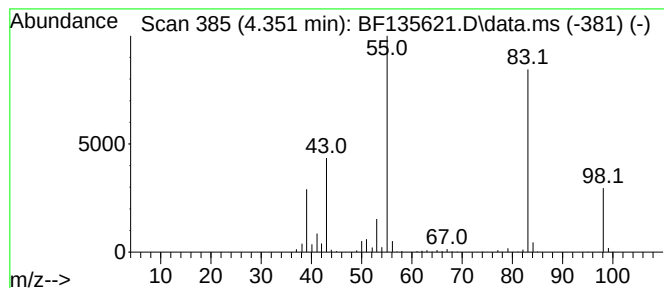
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.351	55.20 ng	2439790	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-			98	C6H10O	000141-79-7	91
2	3-Hexen-2-one			98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-			98	C7H14	004914-91-4	86
4	2-Pentene, 2,4-dimethyl-			98	C7H14	000625-65-0	72
5	Cyclohexane, methyl-			98	C7H14	000108-87-2	64



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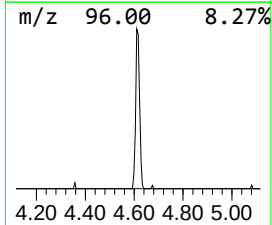
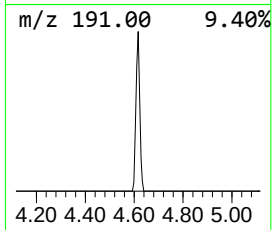
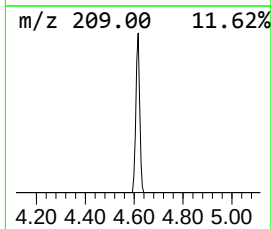
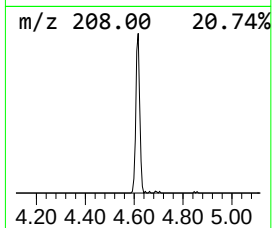
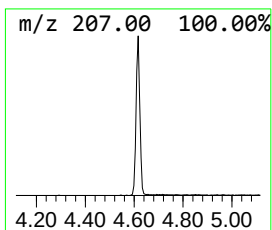
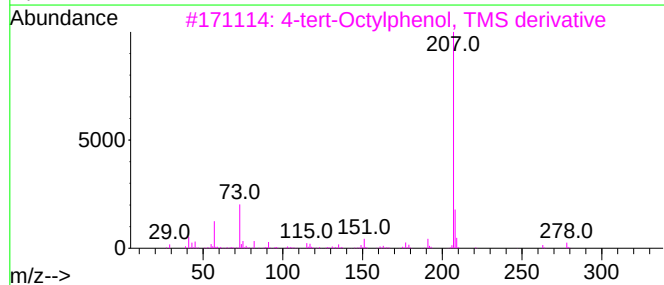
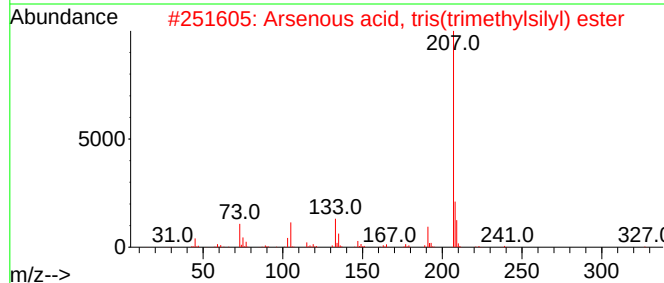
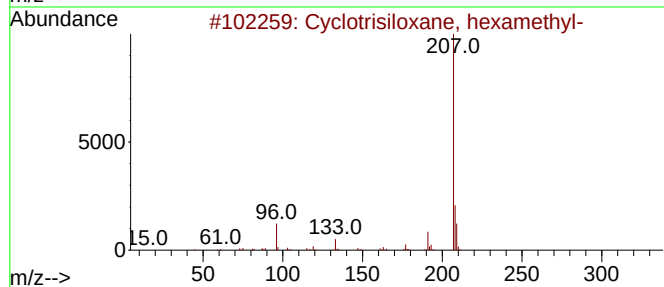
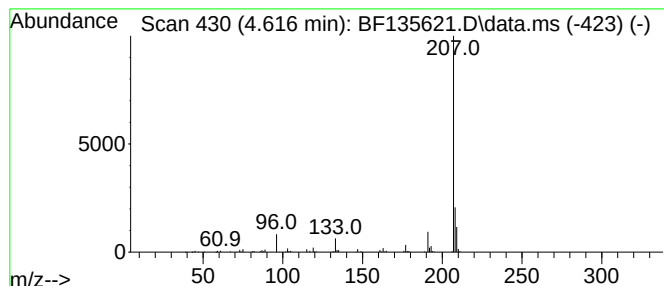
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Cyclotrisiloxane, hexamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.616	4.27 ng	188858	1,4-Dichlorobenzene-d4	6.739

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	64
3			4-tert-Octylphenol, TMS derivative	278	C17H30OSi	078721-87-6	50
4			1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	39
5			Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	39



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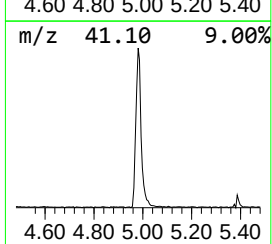
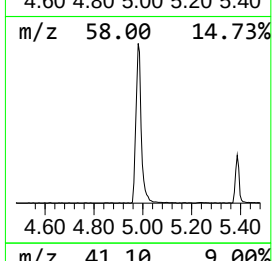
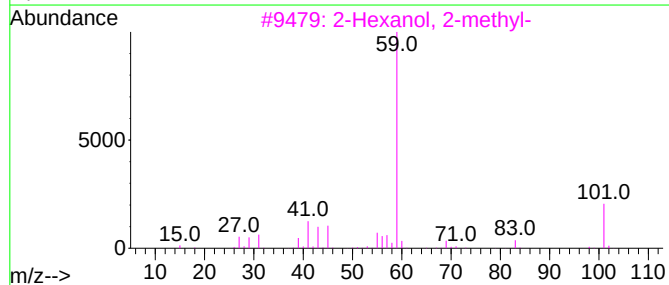
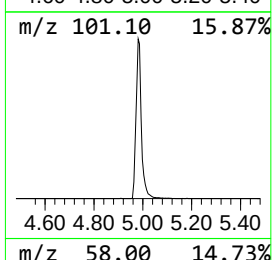
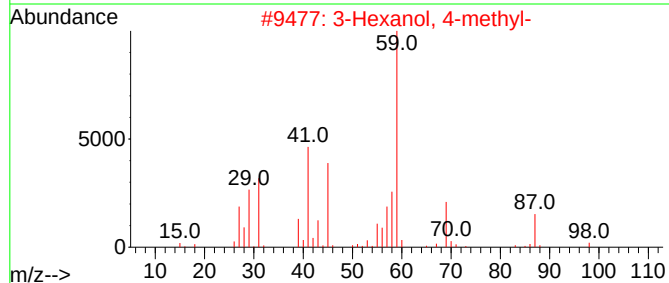
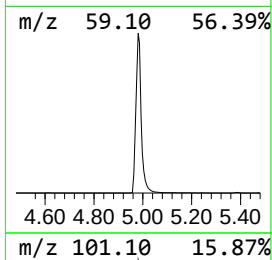
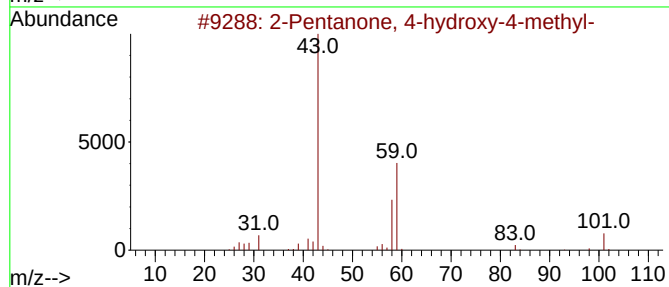
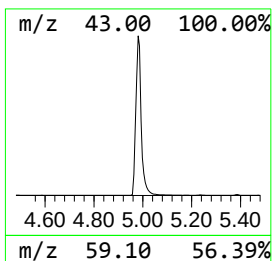
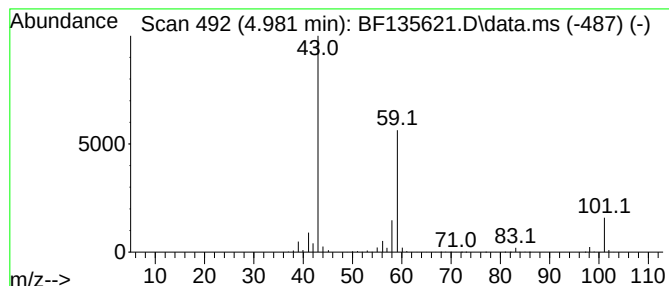
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	51.17 ng	2261560	1,4-Dichlorobenzene-d4	6.739

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
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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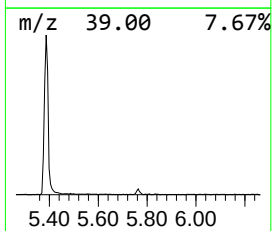
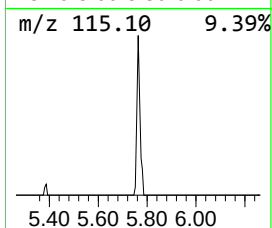
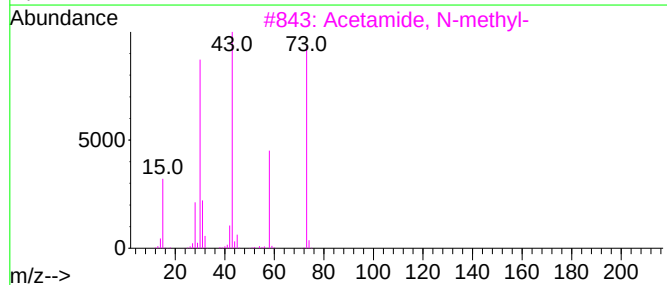
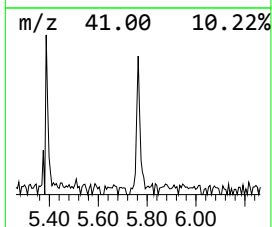
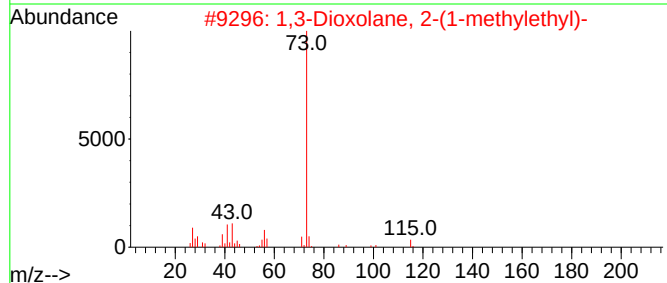
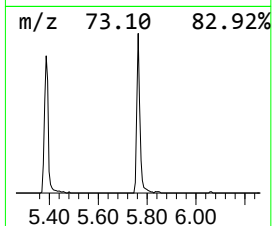
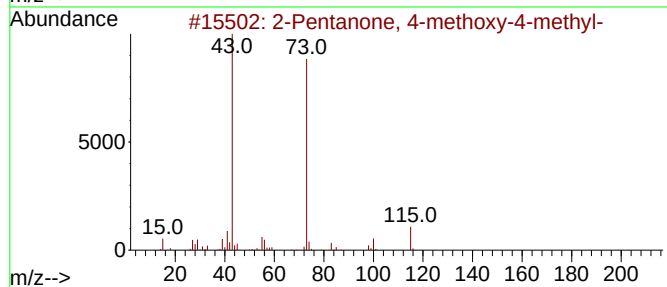
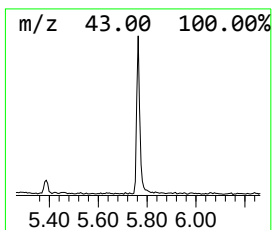
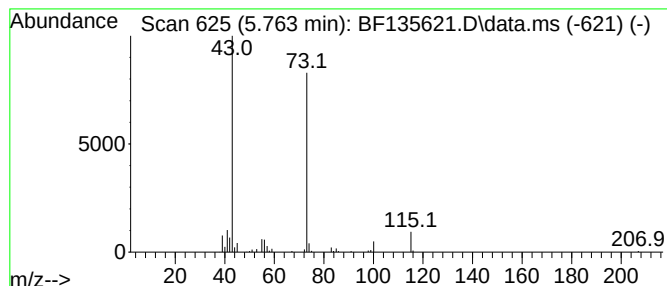
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Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.763	2.09 ng	92582	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	35
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25
5			3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one,...	3.463	27.0	ng	1194660	1	6.739	883979	20.0
3-Penten-2-one,...	4.351	55.2	ng	2439790	1	6.739	883979	20.0
Cyclotrisiloxan...	4.616	4.3	ng	188858	1	6.739	883979	20.0
2-Pentanone, 4-...	4.981	51.2	ng	2261560	1	6.739	883979	20.0
2-Pentanone, 4-...	5.763	2.1	ng	92582	1	6.739	883979	20.0