

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
 Data File : BF136806.D
 Acq On : 28 Dec 2023 21:53
 Operator : CG\JU
 Sample : 06027-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CONTAINMENT

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136806.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	9	13	19	rVB	18211	24974	1.24%	0.207%
2	2.387	45	51	58	rVB2	30356	52081	2.58%	0.431%
3	4.187	354	357	365	rVB	25386	29662	1.47%	0.246%
4	4.257	365	369	377	rBV	36224	43236	2.15%	0.358%
5	4.393	387	392	401	rBV2	98989	150005	7.44%	1.242%
6	4.469	401	405	413	rVB	32610	39418	1.96%	0.326%
7	5.016	493	498	515	rVB	349521	420098	20.85%	3.479%
8	5.422	563	567	574	rBV	1492795	1490700	73.98%	12.344%
9	6.428	733	738	741	rBV	1729777	1580550	78.44%	13.088%
10	6.781	794	798	801	rBV	525349	398895	19.80%	3.303%
11	7.345	889	894	897	rBV	1158282	1055639	52.39%	8.741%
12	8.057	1011	1015	1018	rBV	679670	521504	25.88%	4.318%
13	9.134	1194	1198	1201	rBV	2173804	2014944	100.00%	16.685%
14	9.816	1310	1314	1317	rBV	635245	551121	27.35%	4.564%
15	10.604	1444	1448	1456	rBV	901124	851249	42.25%	7.049%
16	11.304	1563	1567	1571	rBV	610753	497779	24.70%	4.122%
17	11.839	1654	1658	1662	rBV2	38248	43435	2.16%	0.360%
18	12.904	1834	1839	1842	rBV	1599471	1527060	75.79%	12.645%
19	13.857	1995	2001	2003	rBV5	12152	21162	1.05%	0.175%
20	13.957	2012	2018	2025	rBV	358603	365528	18.14%	3.027%
21	15.439	2265	2270	2282	rVB	306165	397588	19.73%	3.292%

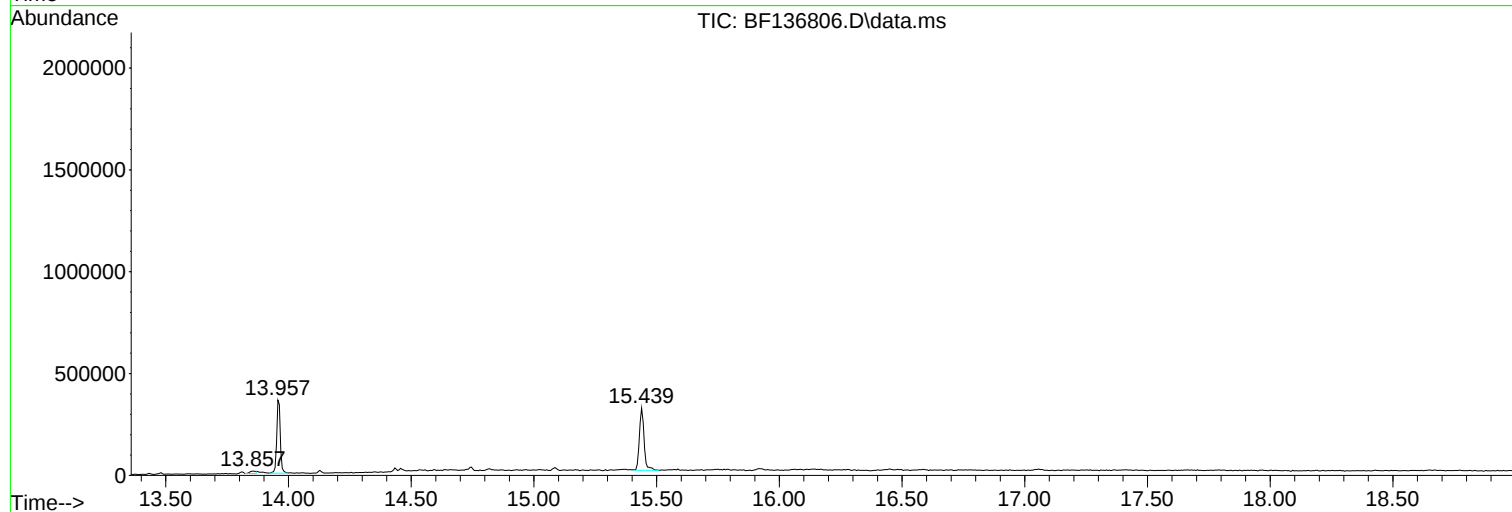
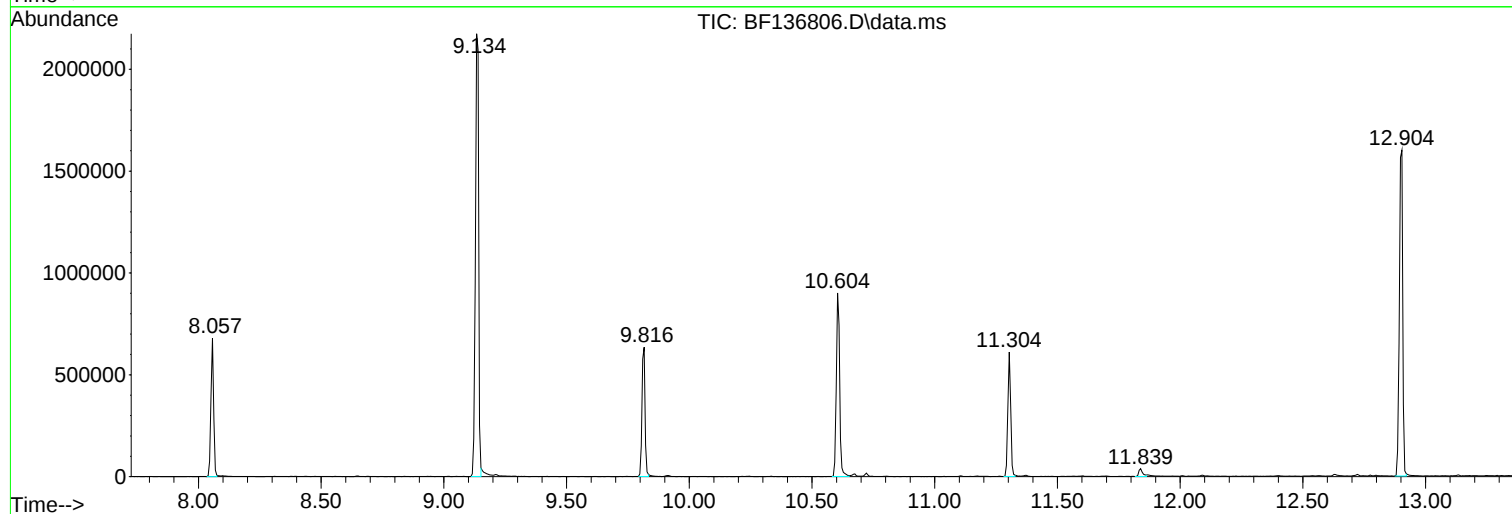
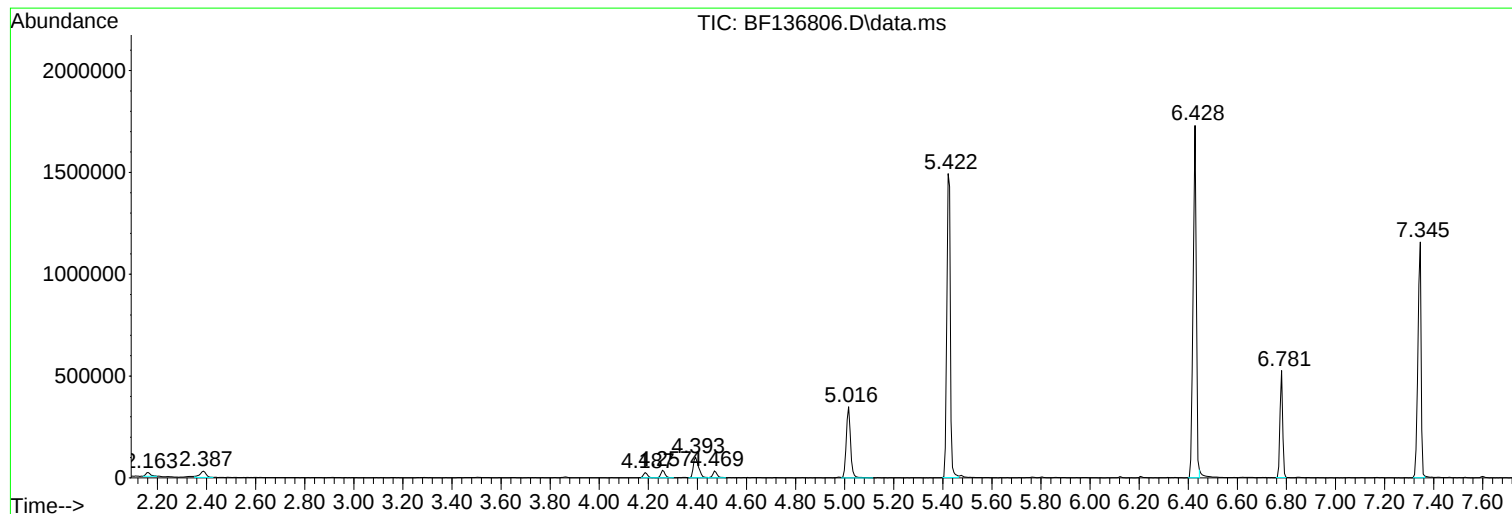
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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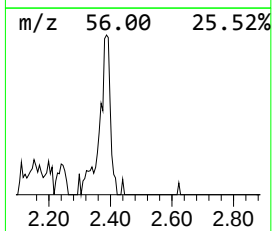
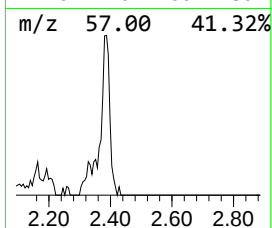
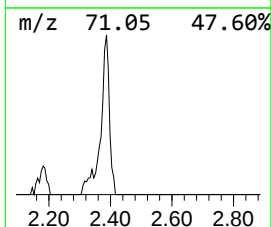
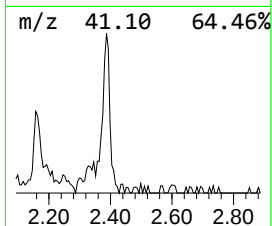
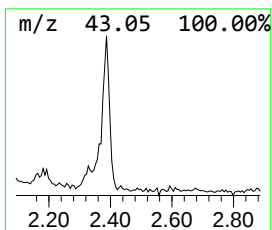
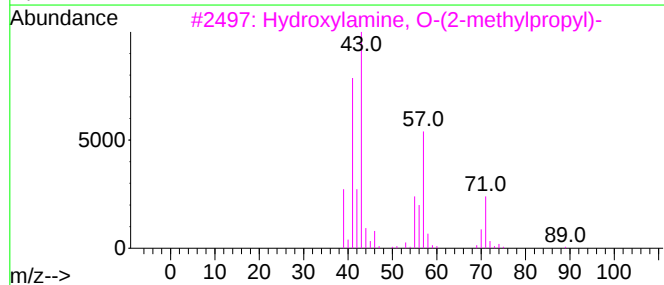
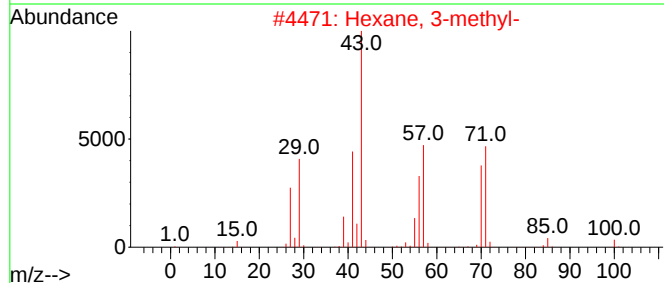
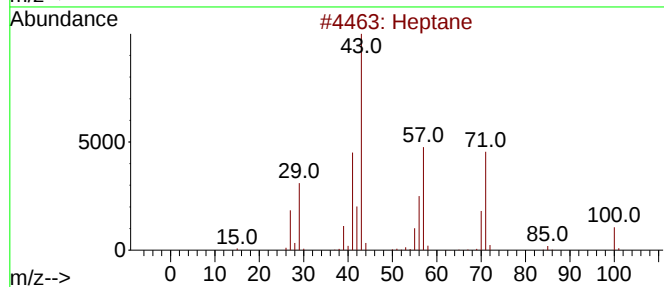
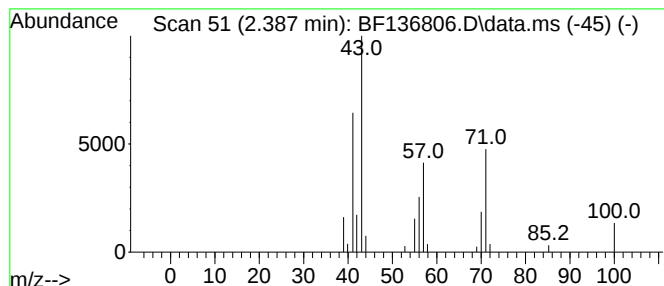
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.387	2.61 ng	52081	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	56
3			Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	47
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	45
5			Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	40



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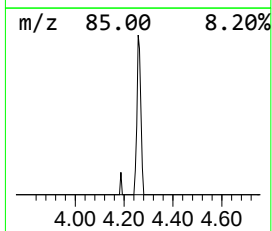
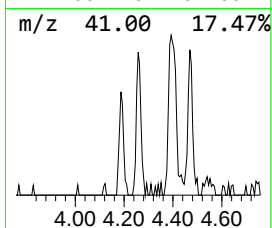
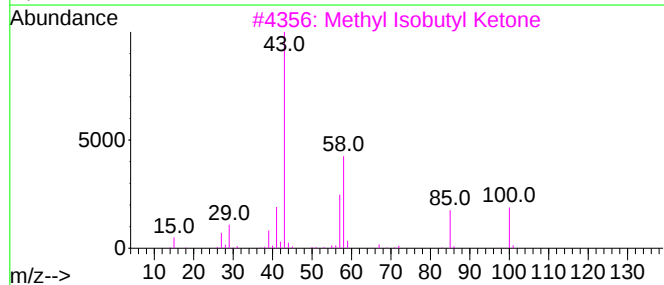
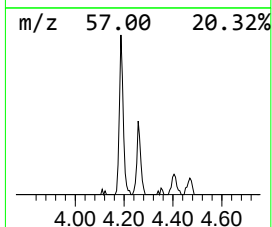
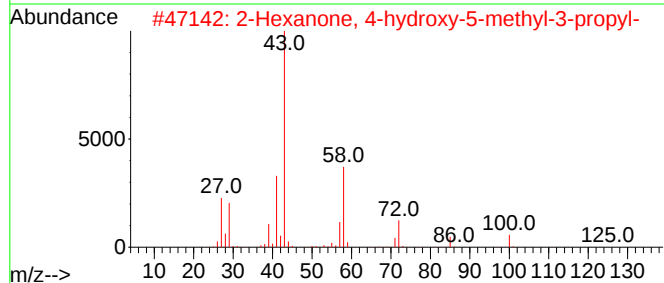
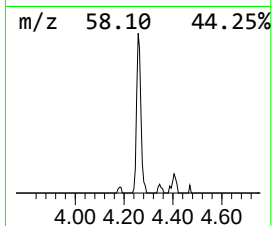
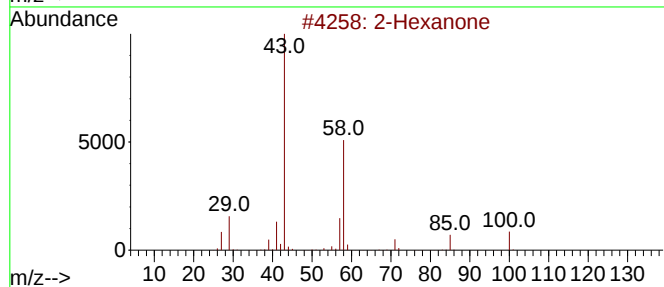
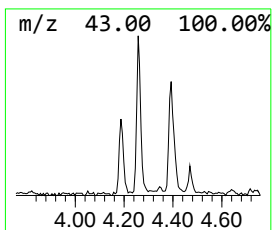
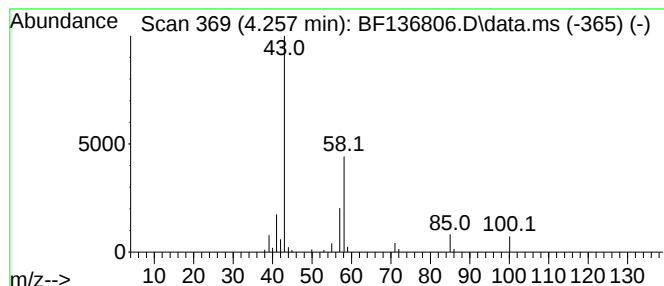
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Hexanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.257	2.17 ng	43236	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone			100	C6H12O	000591-78-6	90
2	2-Hexanone, 4-hydroxy-5-methyl-3...			172	C10H20O2	061141-74-0	83
3	Methyl Isobutyl Ketone			100	C6H12O	000108-10-1	72
4	Oxirane, 2-methyl-2-(1-methyleth...			100	C6H12O	072221-03-5	53
5	2-Hexanone, 5-methyl-			114	C7H14O	000110-12-3	39



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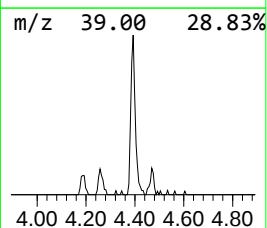
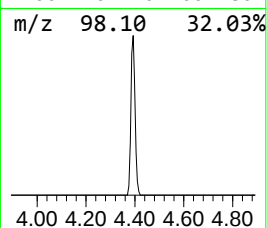
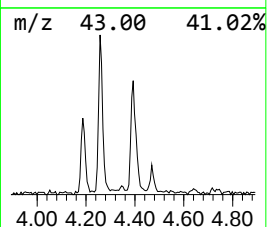
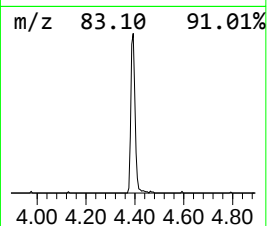
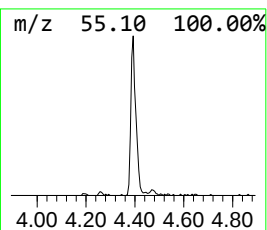
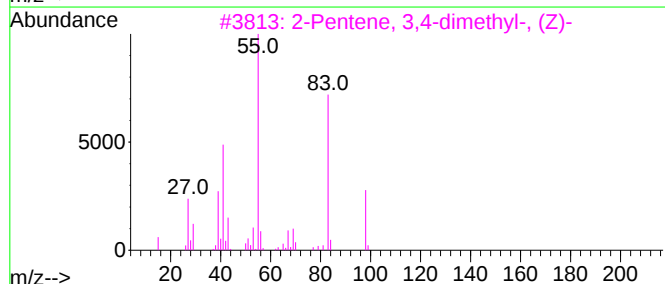
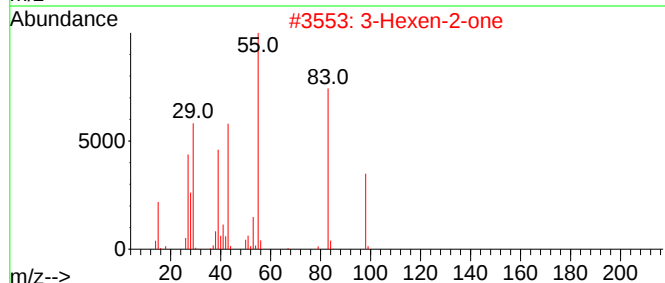
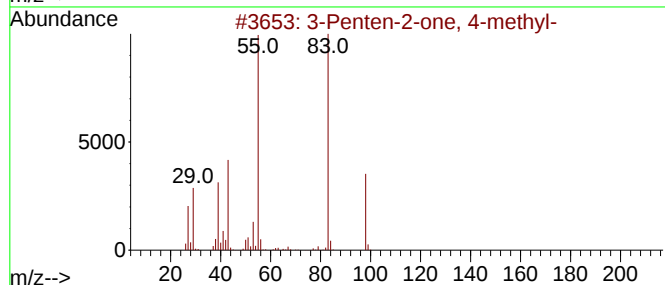
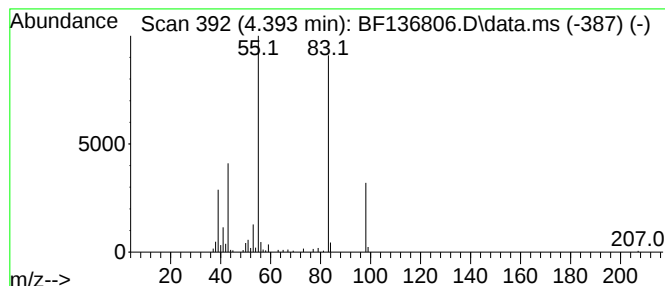
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Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.393	7.52 ng	150005	1,4-Dichlorobenzene-d4	6.781

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-, (Z)-	98	C7H14	004914-91-4	86
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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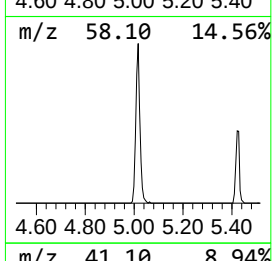
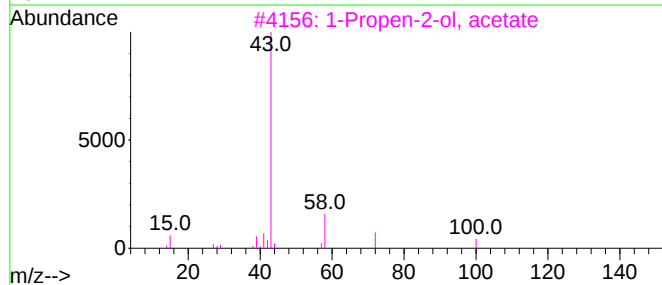
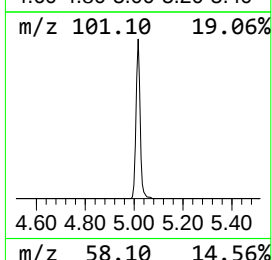
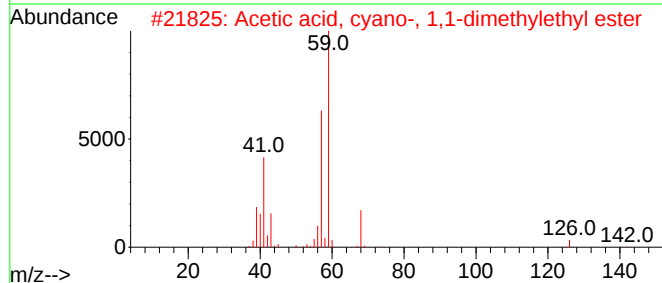
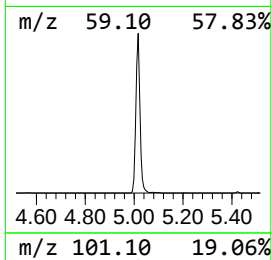
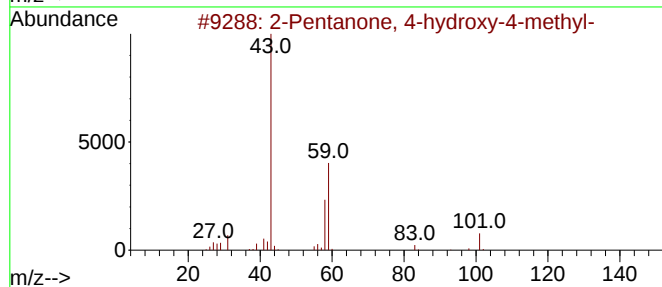
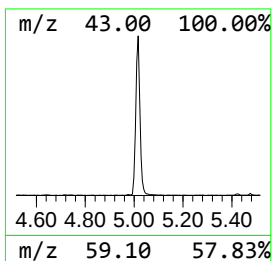
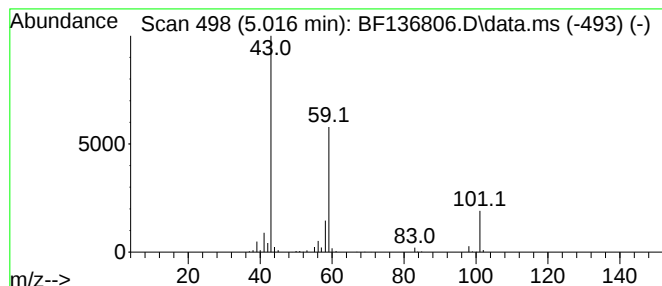
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	21.06 ng	420098	1,4-Dichlorobenzene-d4	6.781

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	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptane	2.387	2.6	ng	52081	1	6.781	398895	20.0
2-Hexanone	4.257	2.2	ng	43236	1	6.781	398895	20.0
3-Penten-2-one,...	4.393	7.5	ng	150005	1	6.781	398895	20.0
2-Pentanone, 4-...	5.016	21.1	ng	420098	1	6.781	398895	20.0