

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
 Data File : BF134315.D
 Acq On : 17 Jul 2023 14:35
 Operator : CG\JU
 Sample : PB154192BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB154192BL

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134315.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.487	403	408	425	rBV	1221377	1410784	33.60%	5.388%
2	5.098	505	512	521	rBV	1409409	2230597	53.12%	8.519%
3	5.487	573	578	581	rBV	2764860	2627826	62.58%	10.036%
4	5.863	639	642	651	rVB	69219	58331	1.39%	0.223%
5	6.481	741	747	750	rBV	2468874	2599601	61.91%	9.928%
6	6.834	804	807	818	rBV	647833	540470	12.87%	2.064%
7	7.404	898	904	907	rBV	1822630	1749343	41.66%	6.681%
8	8.116	1021	1025	1037	rBV	818643	729628	17.38%	2.786%
9	9.192	1202	1208	1211	rBV	3817656	3435484	81.82%	13.120%
10	9.869	1320	1323	1327	rBV	958439	845171	20.13%	3.228%
11	10.669	1454	1459	1462	rBV	2848500	2561601	61.01%	9.783%
12	11.369	1574	1578	1581	rBV	1116237	968132	23.06%	3.697%
13	12.968	1845	1850	1853	rBV	4211670	4198894	100.00%	16.036%
14	14.027	2026	2030	2039	rBV	1020059	894617	21.31%	3.417%
15	14.810	2158	2163	2171	rBV	39160	44874	1.07%	0.171%
16	15.157	2218	2222	2227	rVB	50407	57969	1.38%	0.221%
17	15.527	2280	2285	2299	rBV	613888	939226	22.37%	3.587%
18	16.004	2361	2366	2374	rVB	52477	85707	2.04%	0.327%
19	16.539	2451	2457	2464	rBV2	48451	84806	2.02%	0.324%
20	17.168	2556	2564	2574	rBV3	26853	67321	1.60%	0.257%
21	17.921	2683	2692	2703	rBV6	16505	54037	1.29%	0.206%

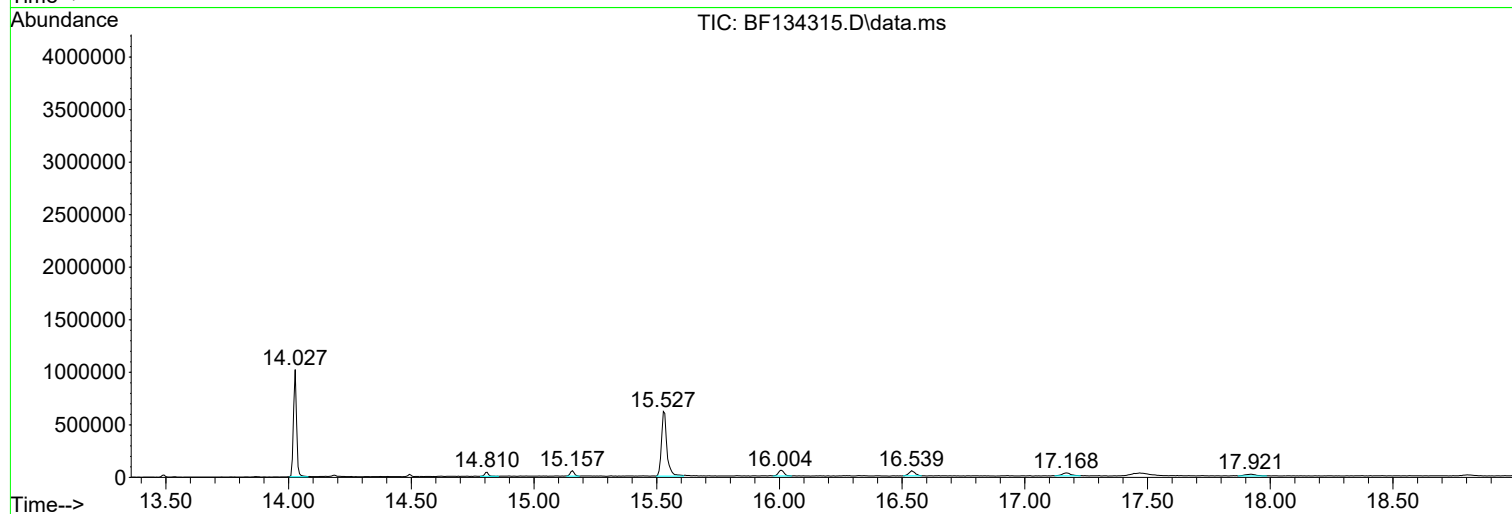
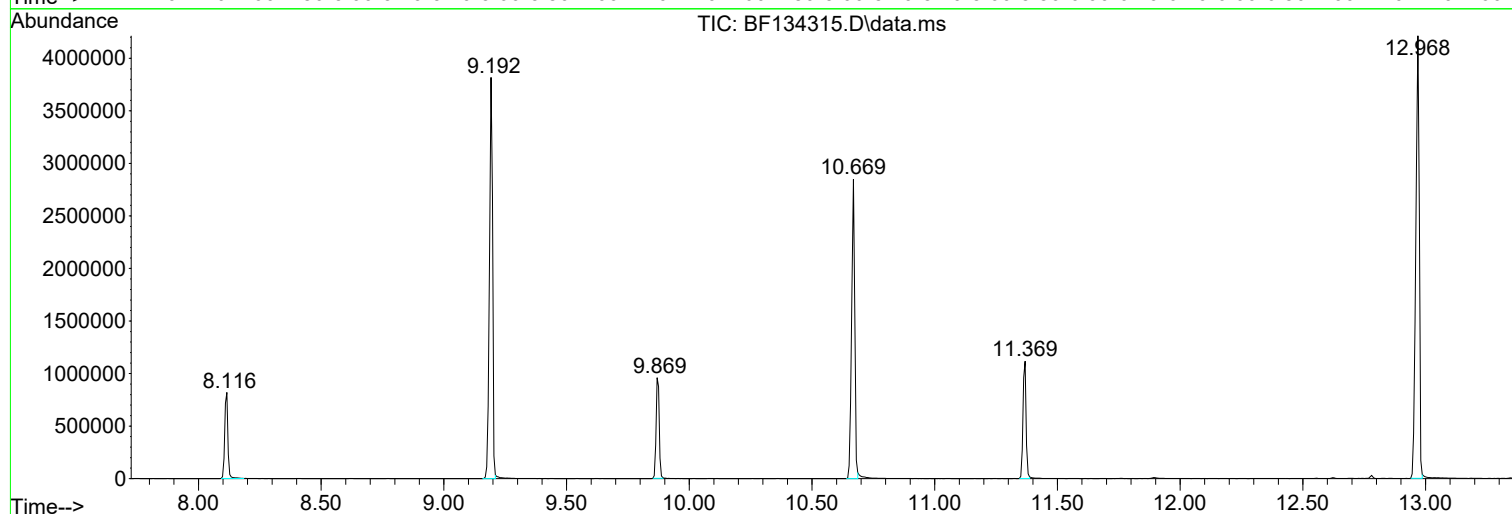
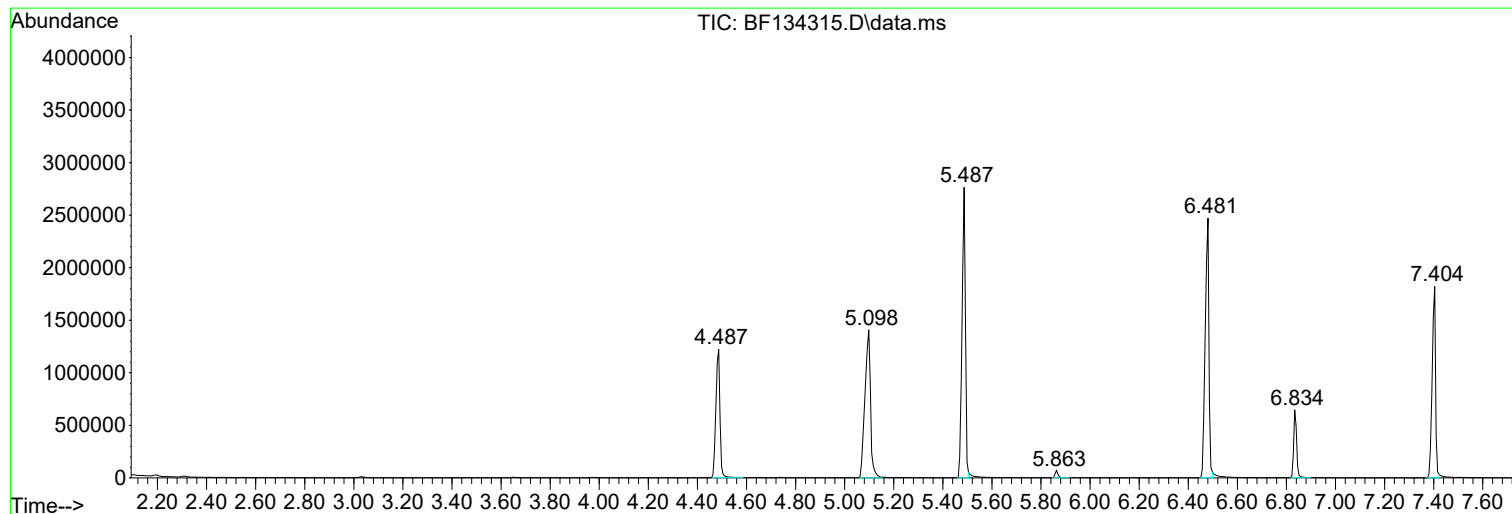
Sum of corrected areas: 26184419

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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Instrument :
BNA_F
ClientSampleId :
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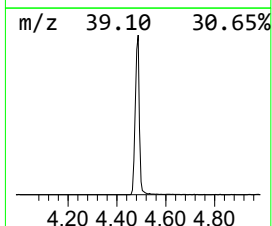
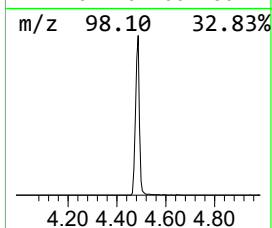
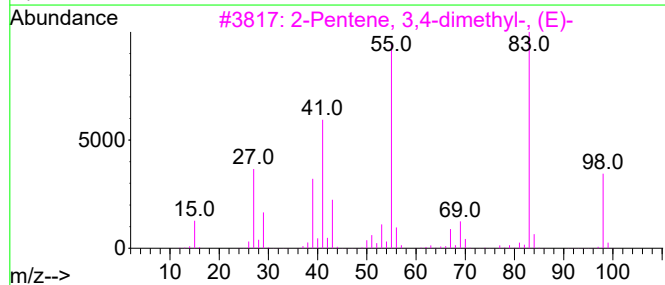
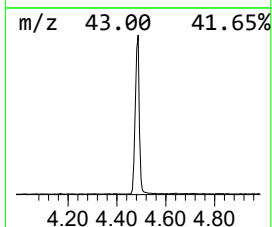
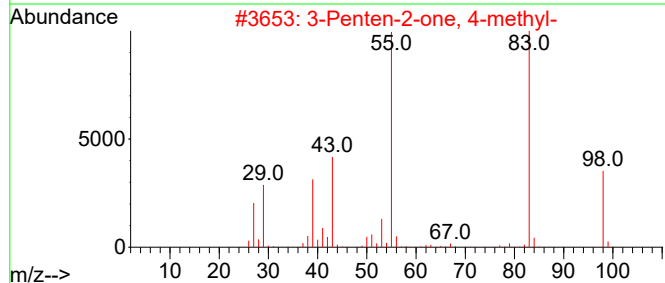
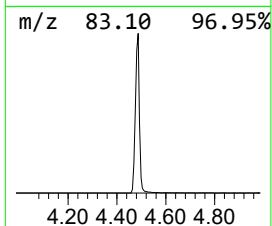
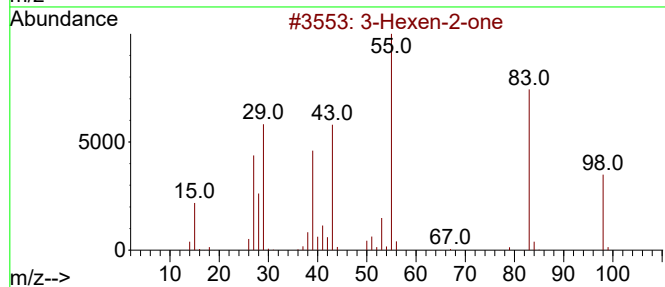
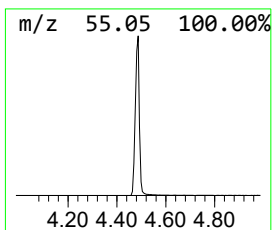
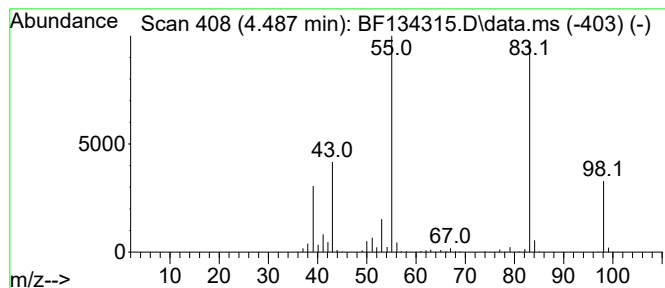
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.487	52.21 ng	1410780	1,4-Dichlorobenzene-d4	6.834

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	90
4			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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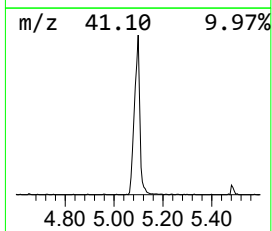
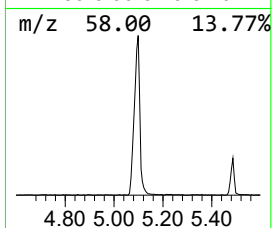
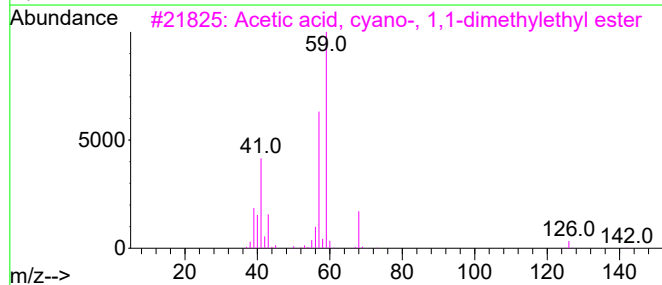
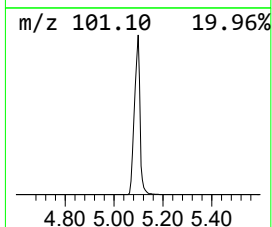
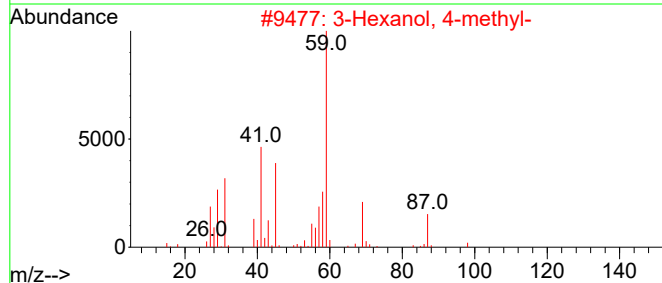
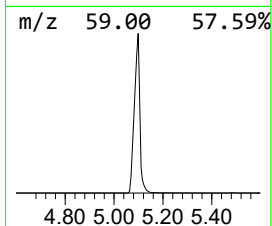
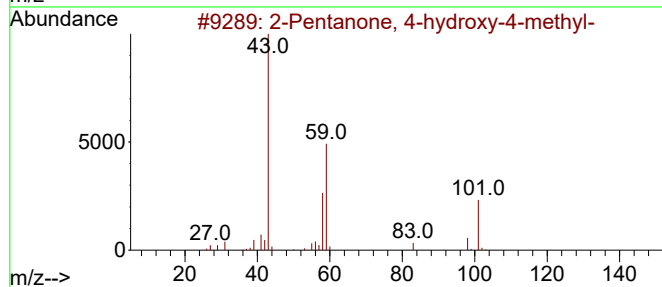
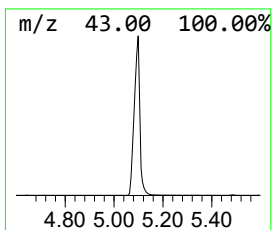
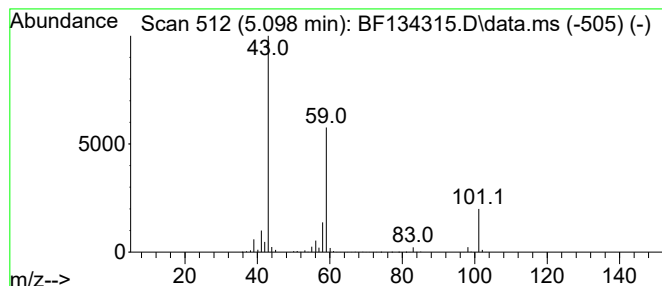
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.098	82.54 ng	2230600	1,4-Dichlorobenzene-d4	6.834	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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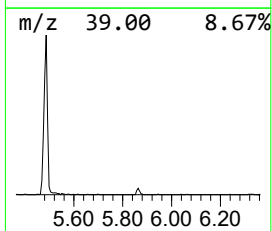
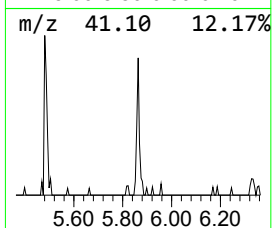
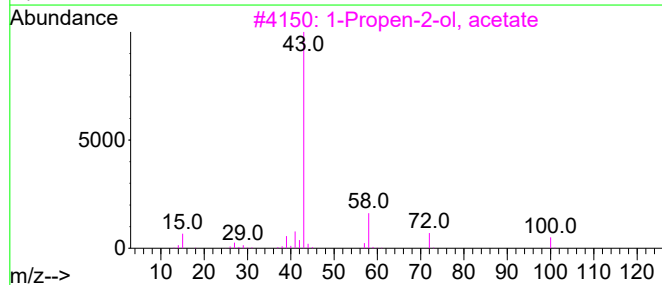
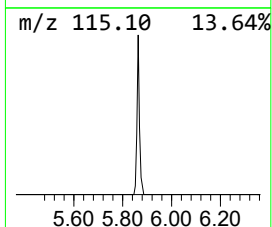
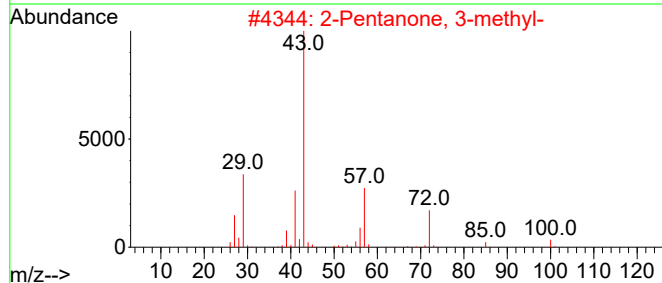
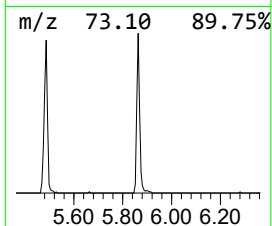
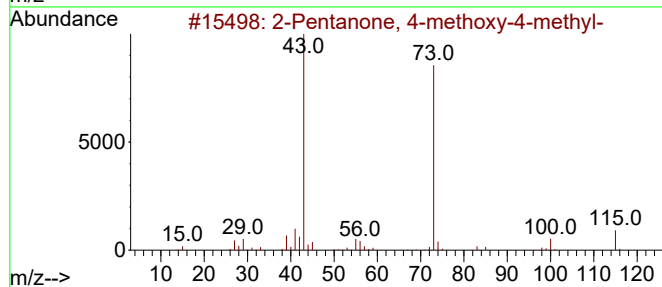
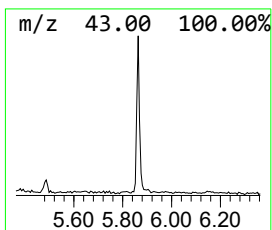
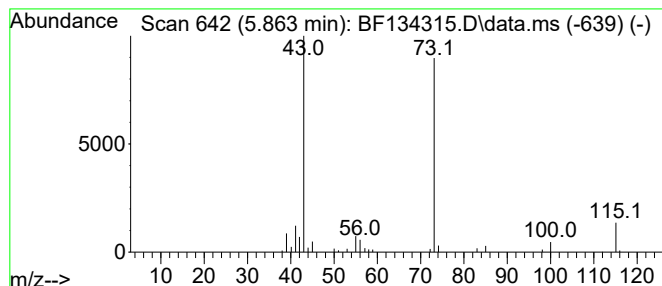
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.863	2.16 ng	58331	1,4-Dichlorobenzene-d4			6.834
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-		130	C7H14O2	000107-70-0	90
2	2-Pentanone, 3-methyl-		100	C6H12O	000565-61-7	27
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
4	N-Formylmorpholine		115	C5H9NO2	004394-85-8	10
5	1-Amino-3,3-dimethyl-2-butanone		115	C6H13NO	082962-91-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.487	52.2	ng	1410780	1	6.834	540470	20.0
2-Pentanone, 4-...	5.098	82.5	ng	2230600	1	6.834	540470	20.0
2-Pentanone, 4-...	5.863	2.2	ng	58331	1	6.834	540470	20.0