

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030323\
 Data File : BF132626.D
 Acq On : 03 Mar 2023 13:42
 Operator : CG\JU
 Sample : PB151190BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB151190BL

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: BF132626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.640	345	349	356	rBV	208194	230402	3.09%	0.503%
2	5.245	445	452	464	rVB	2334529	3433191	46.02%	7.489%
3	5.634	513	518	521	rBV	5016360	5144289	68.96%	11.221%
4	6.016	579	583	590	rBV	176476	142986	1.92%	0.312%
5	6.628	681	687	690	rBV	4535473	5149688	69.03%	11.233%
6	6.998	746	750	753	rBV	1585167	1255411	16.83%	2.738%
7	7.569	841	847	850	rBV	3298849	3527267	47.28%	7.694%
8	8.286	965	969	972	rBV	1981116	1633833	21.90%	3.564%
9	9.363	1147	1152	1155	rBV	6724512	6155894	82.52%	13.428%
10	10.045	1264	1268	1272	rBV	2371023	1957738	26.24%	4.270%
11	10.845	1399	1404	1407	rBV	4216721	4233400	56.75%	9.234%
12	11.545	1519	1523	1526	rBV	2336005	2126202	28.50%	4.638%
13	13.139	1789	1794	1797	rBV	7384415	7459593	100.00%	16.271%
14	14.204	1971	1975	1979	rBV	2127179	1877943	25.17%	4.096%
15	15.757	2233	2239	2250	rBV	1099601	1517063	20.34%	3.309%

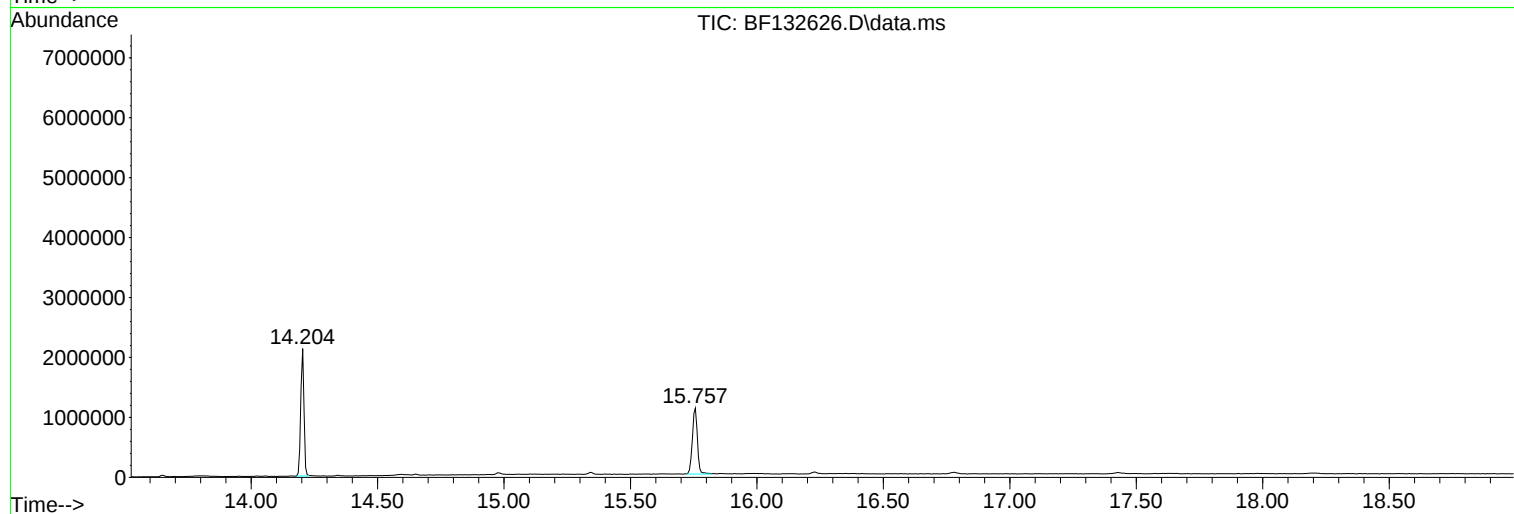
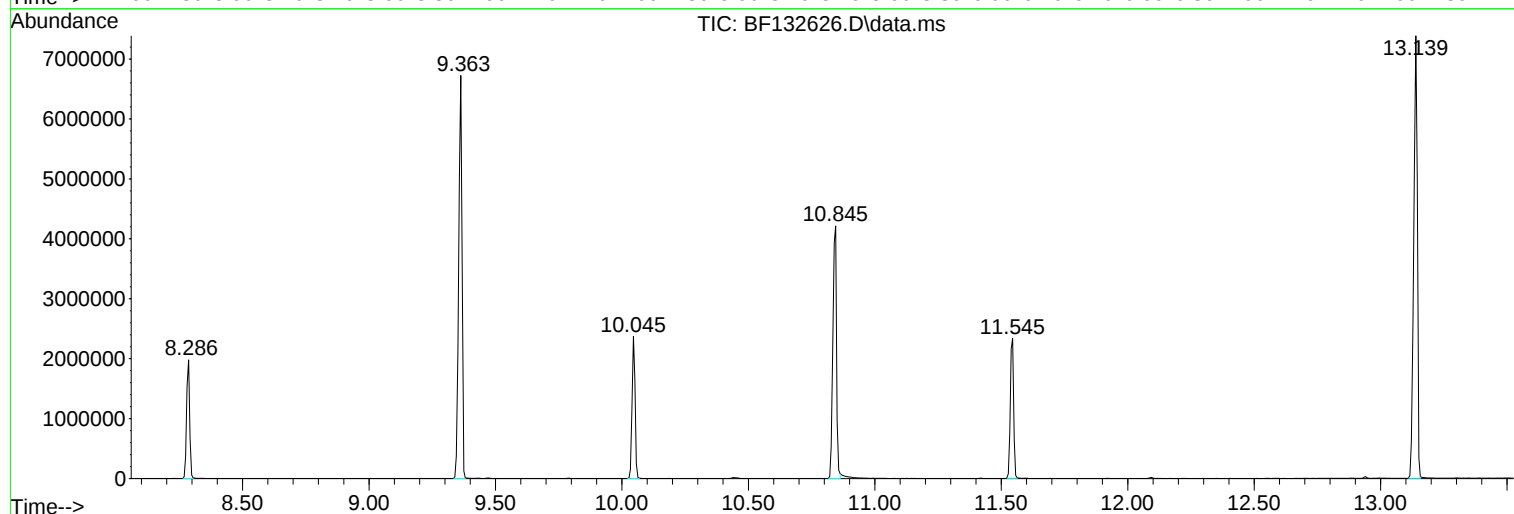
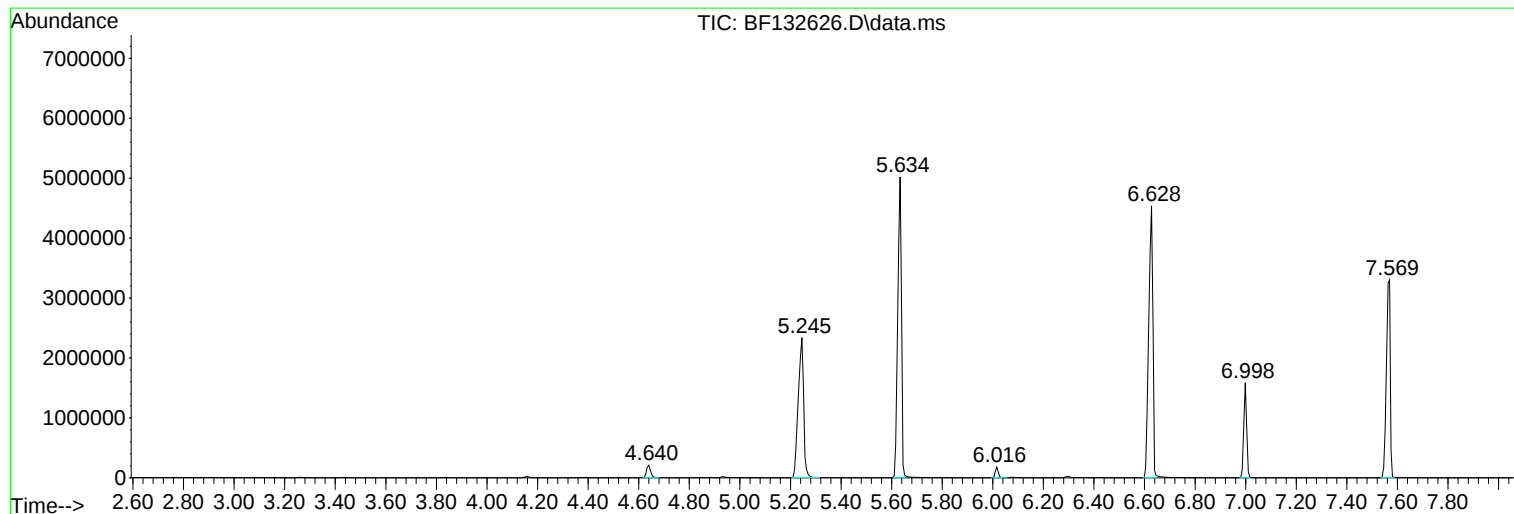
Sum of corrected areas: 45844900

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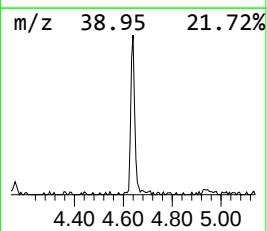
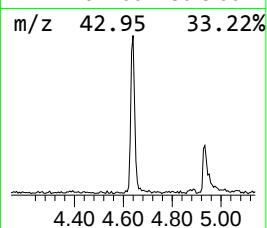
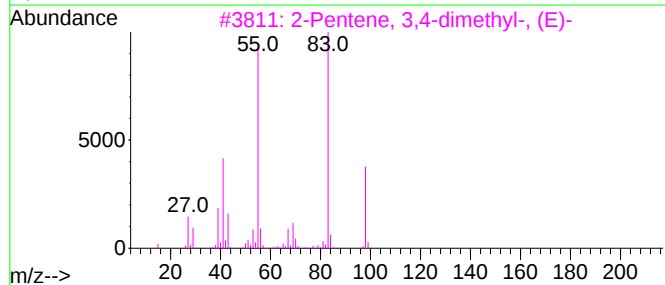
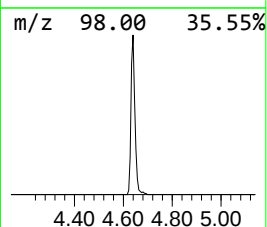
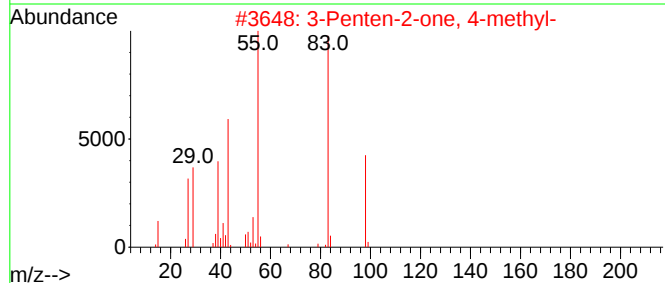
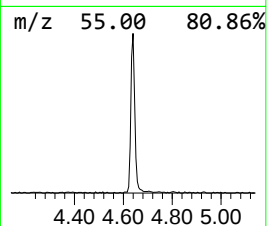
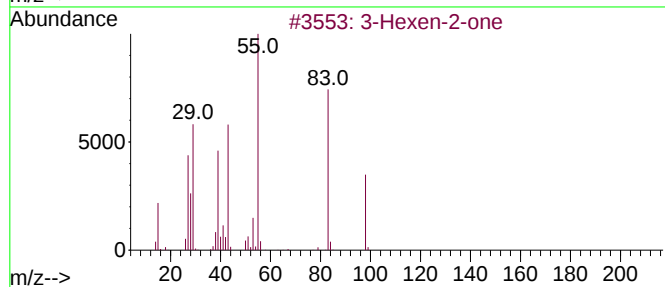
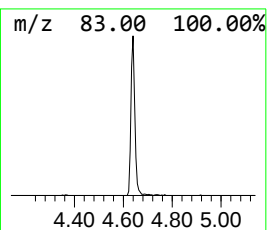
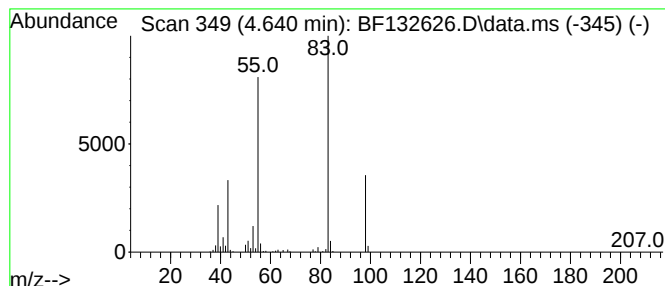
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.640	3.67 ng	230402	1,4-Dichlorobenzene-d4	6.998

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			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	83
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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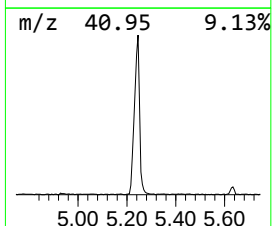
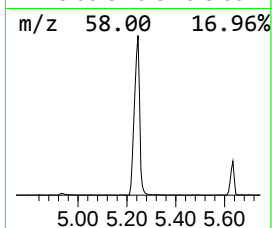
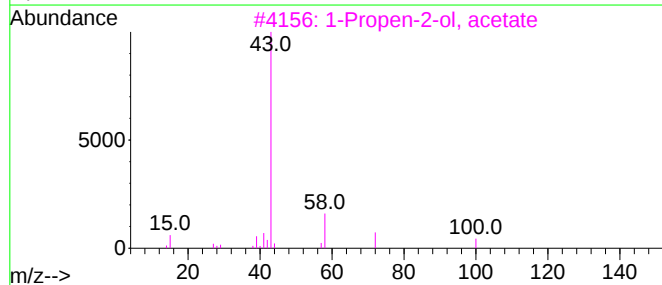
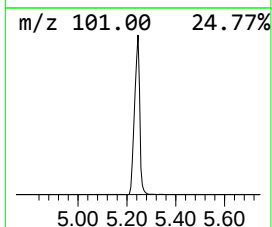
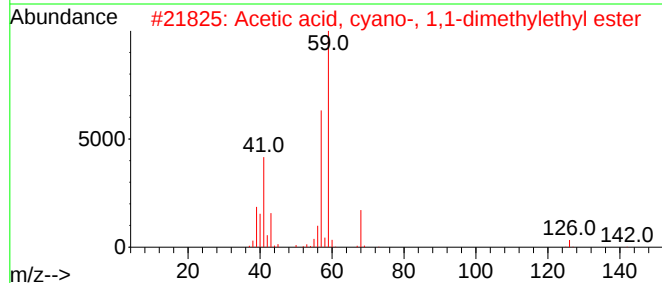
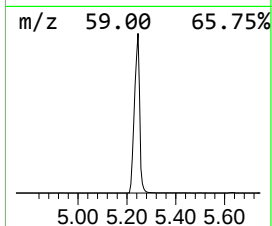
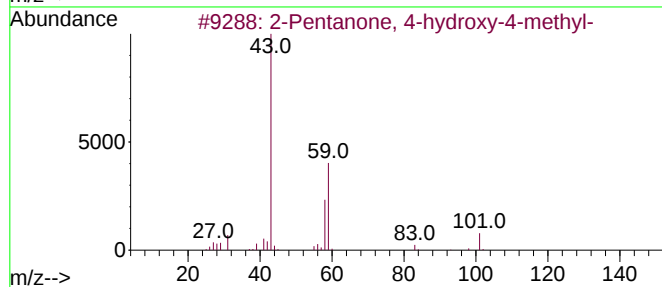
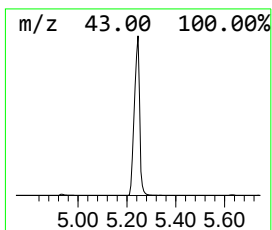
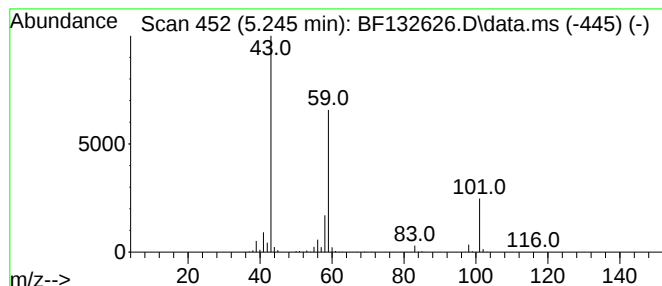
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.245	54.69 ng	3433190	1,4-Dichlorobenzene-d4	6.998

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			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Acetone	58	C3H6O	000067-64-1	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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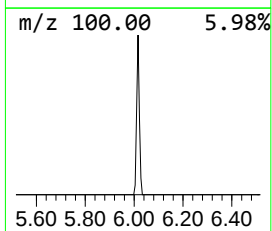
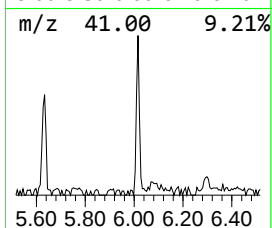
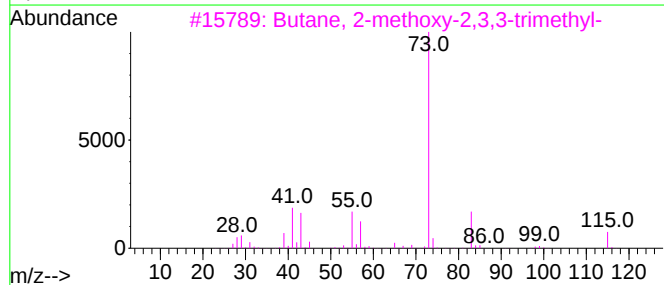
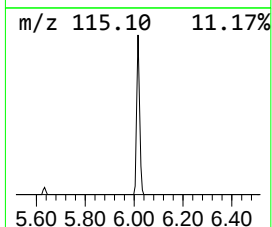
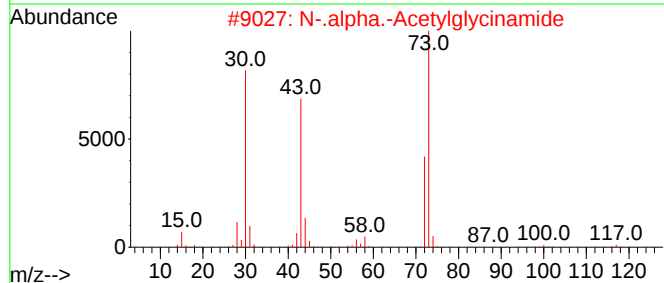
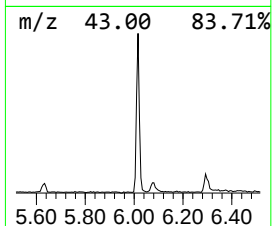
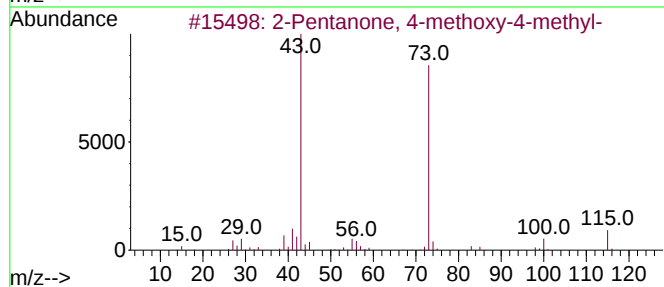
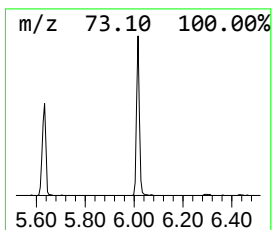
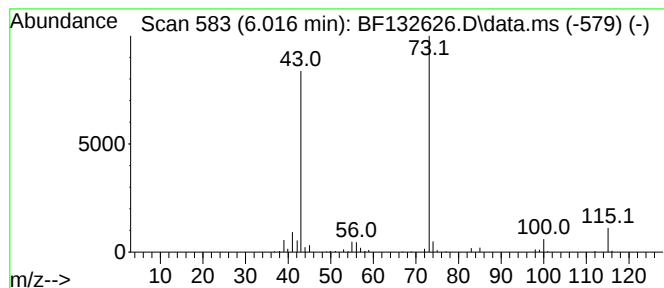
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.016	2.28 ng	142986	1,4-Dichlorobenzene-d4	6.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83		
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	40		
3	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23		
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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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	4.640	3.7	ng	230402	1	6.998	1255410	20.0
2-Pentanone, 4-...	5.245	54.7	ng	3433190	1	6.998	1255410	20.0
2-Pentanone, 4-...	6.016	2.3	ng	142986	1	6.998	1255410	20.0