

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102623\
 Data File : BF135959.D
 Acq On : 26 Oct 2023 12:47
 Operator : CG\JU
 Sample : PB156430BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB156430BL

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-BF102523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135959.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	16	24	29	rVB	87602	124550	1.72%	0.245%
2	3.645	259	265	272	rVB	95179	130047	1.79%	0.256%
3	4.481	400	407	410	rBV	2907354	3430757	47.32%	6.753%
4	5.087	501	510	524	rBV	2259682	4088077	56.39%	8.046%
5	5.475	569	576	579	rBV	5079314	6184996	85.31%	12.174%
6	5.851	636	640	643	rBV	243589	184181	2.54%	0.363%
7	6.457	736	743	746	rBV	4525685	6207510	85.62%	12.218%
8	6.822	801	805	808	rBV	1308938	996576	13.75%	1.962%
9	7.386	894	901	904	rBV	3393035	3919276	54.06%	7.714%
10	8.104	1017	1023	1026	rBV	1642803	1400552	19.32%	2.757%
11	9.186	1200	1207	1210	rBV	6755992	6782149	93.55%	13.349%
12	9.863	1315	1322	1325	rBV	1766706	1588915	21.92%	3.127%
13	10.657	1446	1457	1460	rBV	4070123	4116141	56.77%	8.102%
14	11.351	1571	1575	1578	rBV	2016601	1637046	22.58%	3.222%
15	12.786	1815	1819	1824	rVB	155106	140986	1.94%	0.277%
16	12.957	1843	1848	1851	rBV	6353066	7250041	100.00%	14.270%
17	13.492	1937	1939	1944	rBV	91551	80511	1.11%	0.158%
18	14.004	2022	2026	2030	rBV	1650270	1423019	19.63%	2.801%
19	15.492	2273	2279	2288	rBV	890724	1120726	15.46%	2.206%

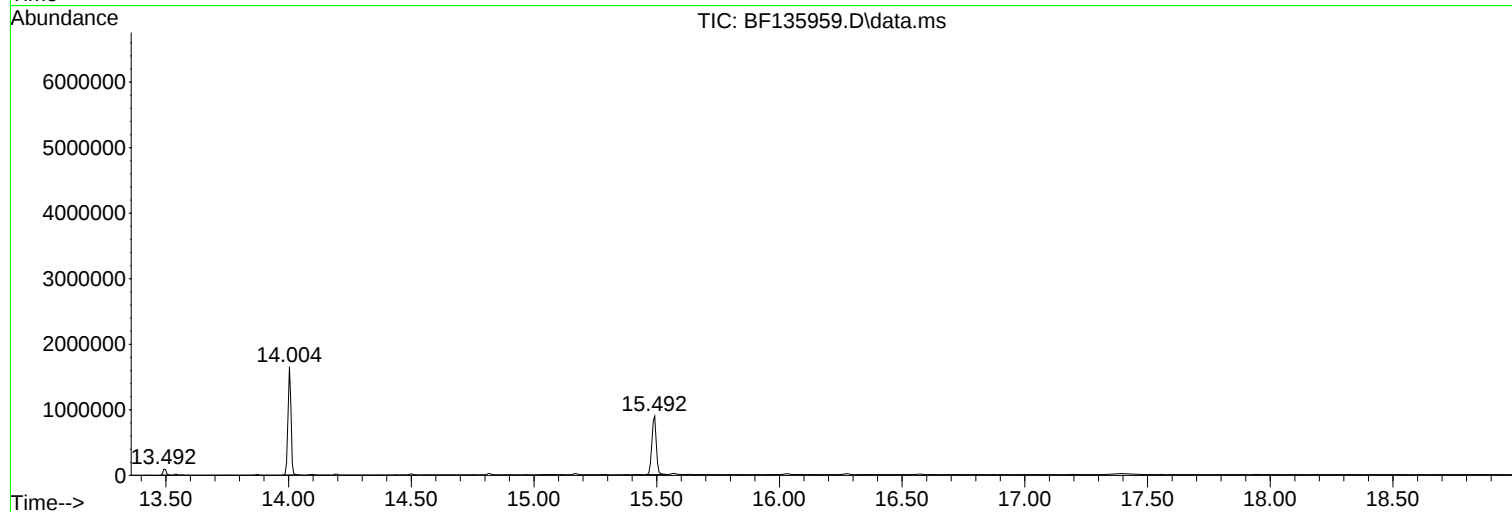
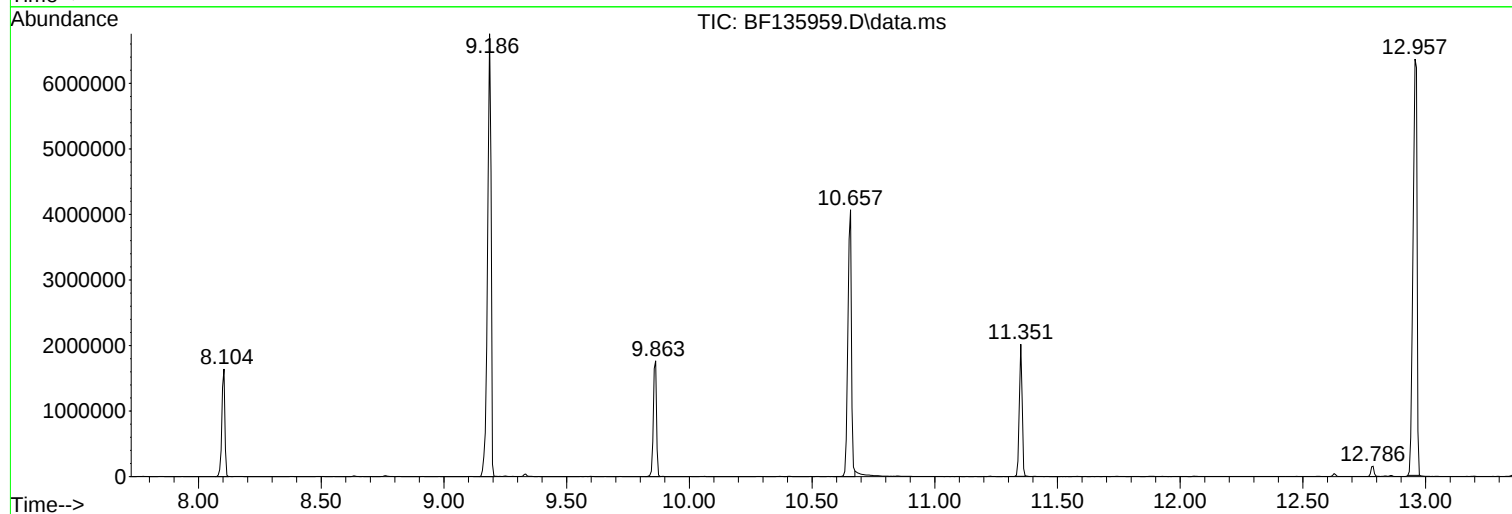
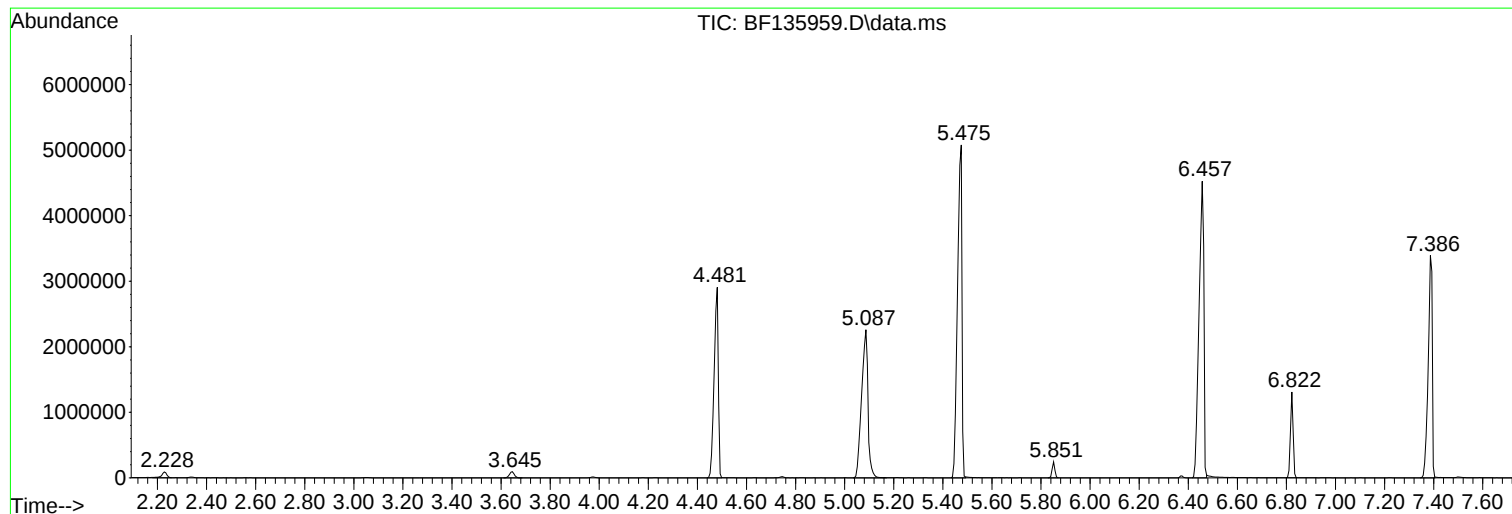
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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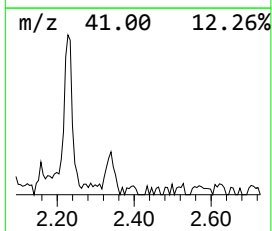
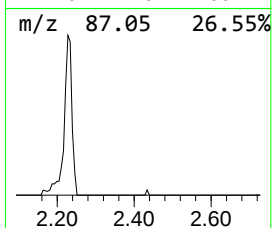
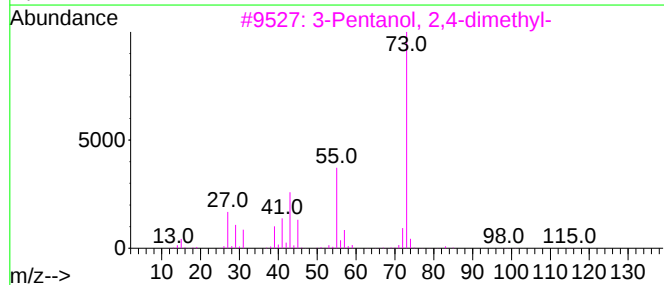
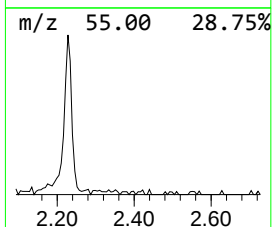
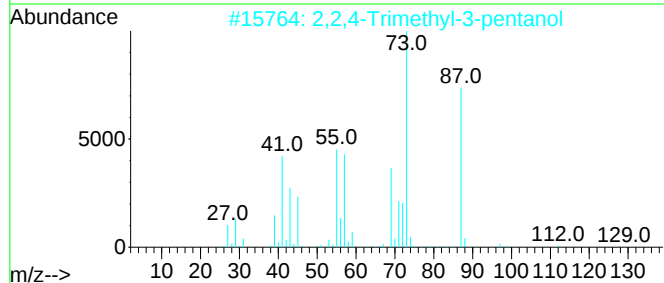
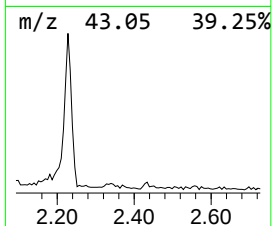
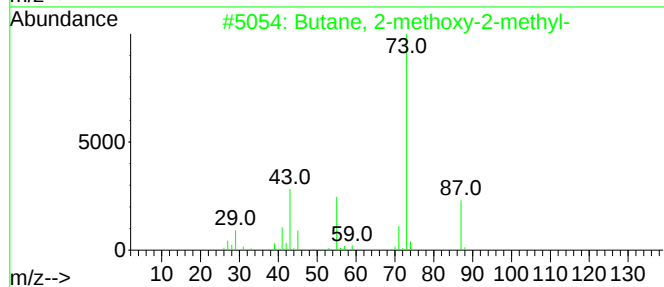
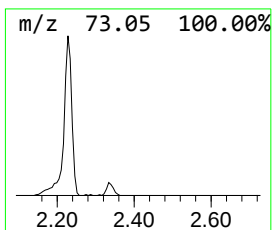
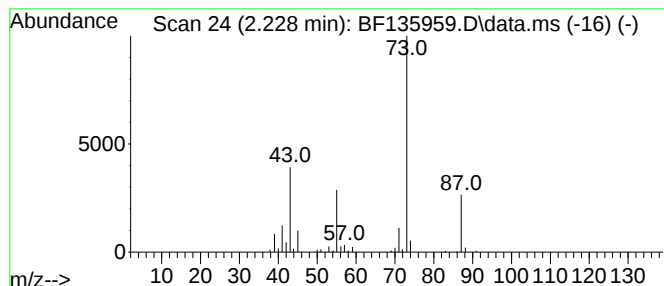
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	2.50 ng	124550	1,4-Dichlorobenzene-d4	6.822

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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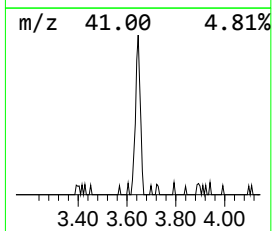
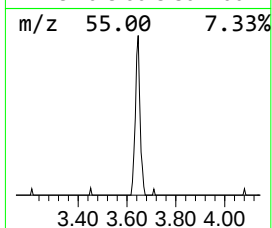
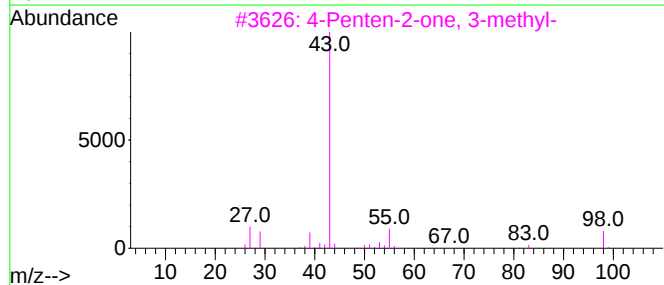
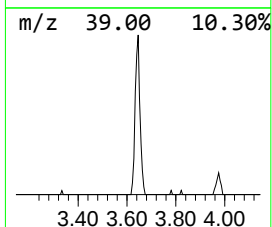
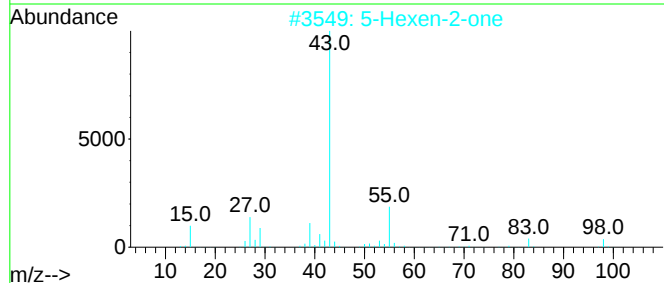
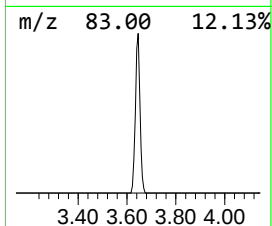
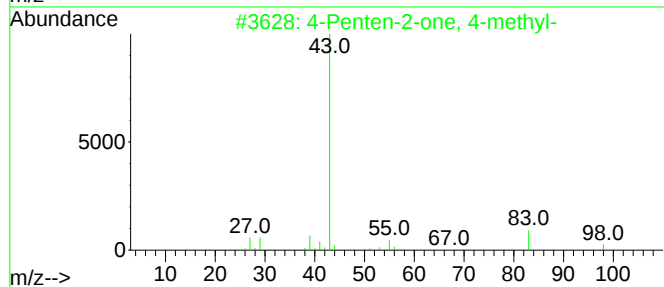
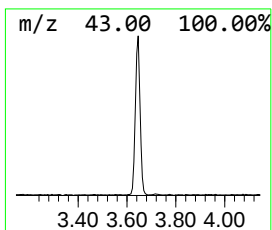
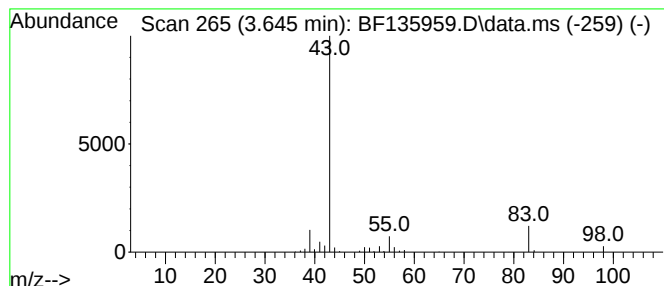
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.645	2.61 ng	130047	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2			5-Hexen-2-one	98	C6H10O	000109-49-9	50
3			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	28
4			2-Vinylethyl acetate	114	C6H10O2	001576-84-7	23
5			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	23



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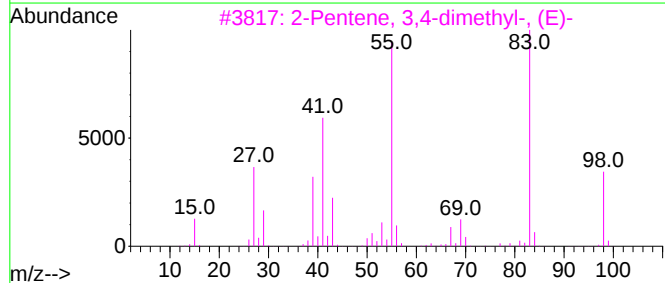
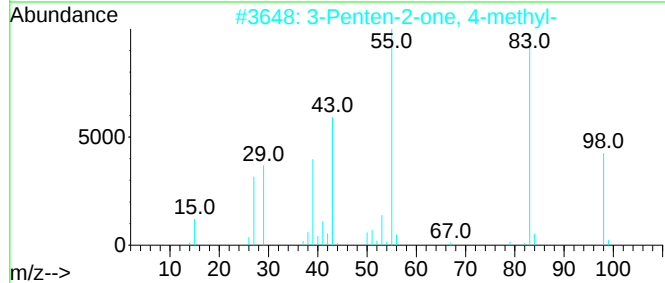
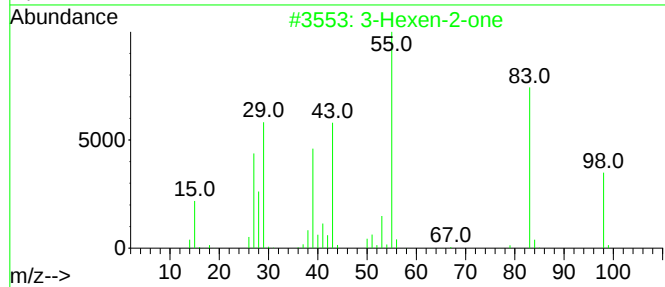
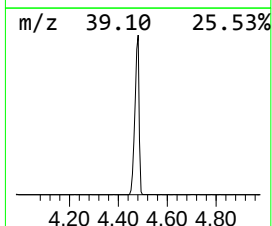
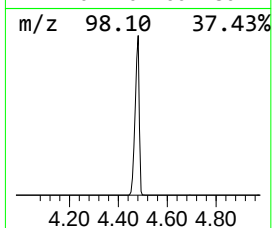
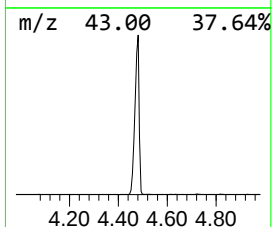
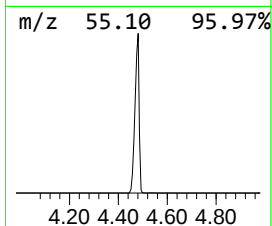
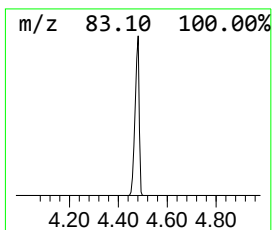
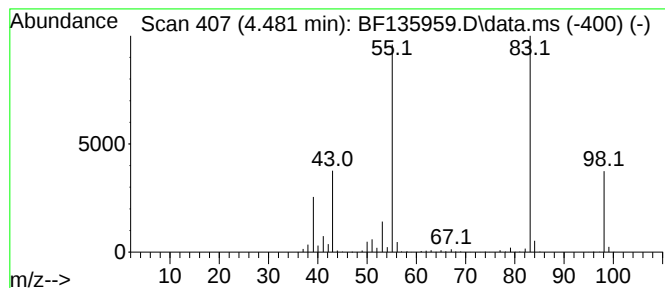
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	68.85 ng	3430760	1,4-Dichlorobenzene-d4	6.822

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



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ALS Vial : 3 Sample Multiplier: 1

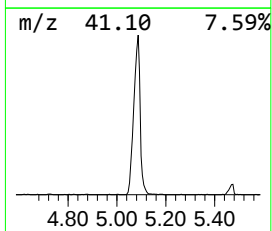
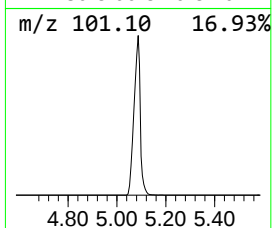
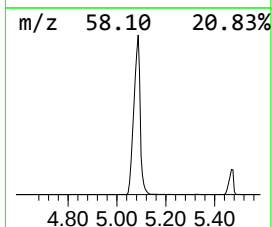
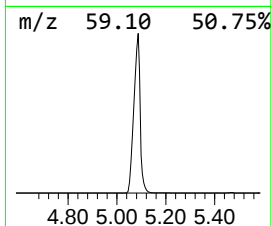
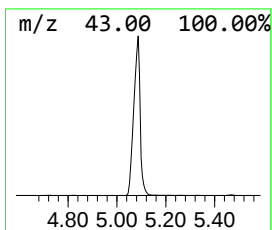
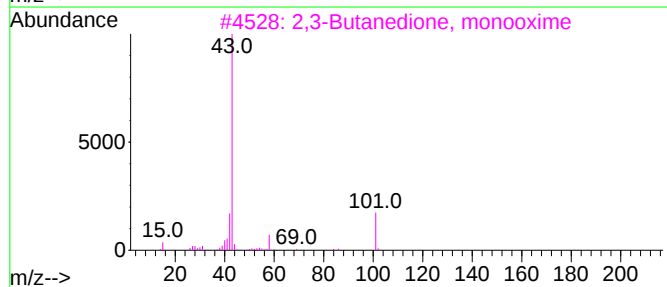
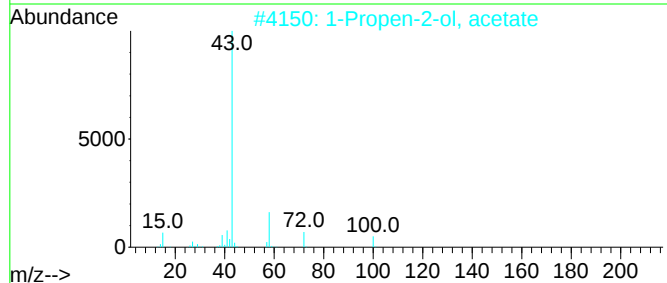
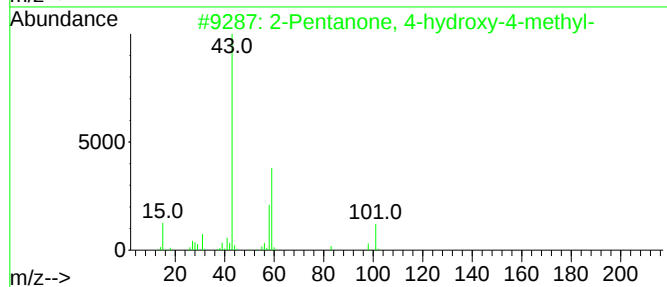
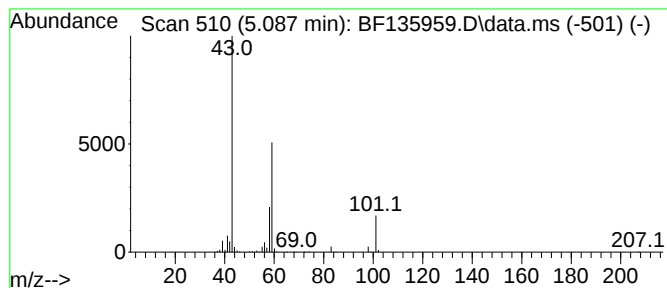
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.087	82.04 ng	4088080	1,4-Dichlorobenzene-d4			6.822
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	83
2	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	12
4	Formamide, N,N-diethyl-		101	C5H11NO	000617-84-5	9
5	Acetone		58	C3H6O	000067-64-1	9



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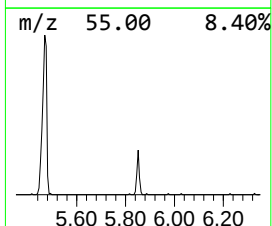
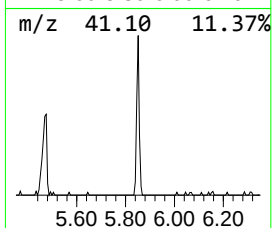
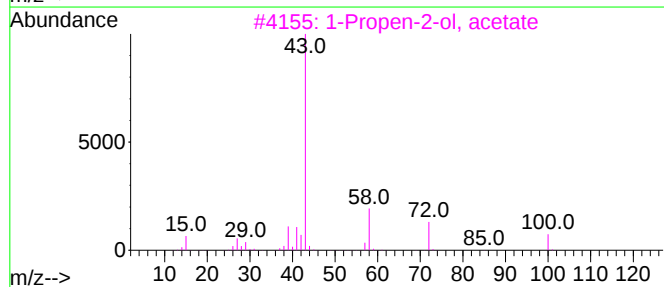
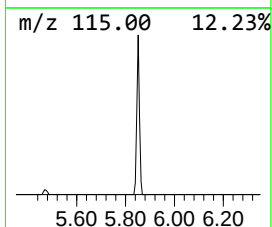
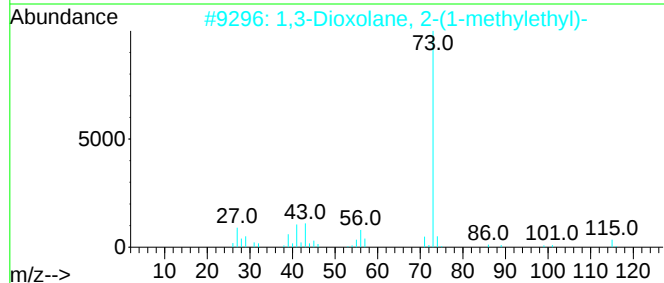
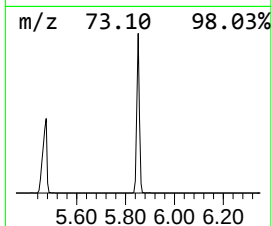
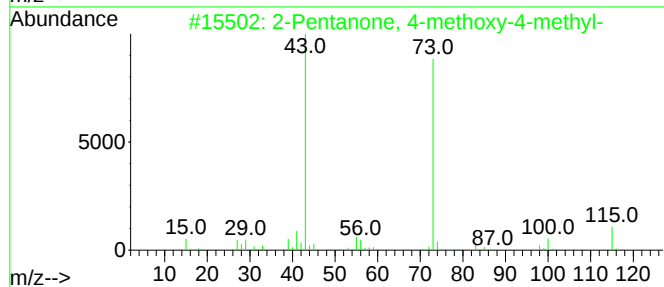
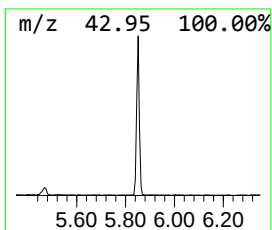
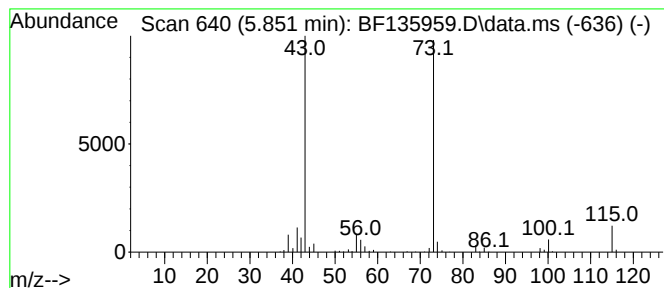
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.851	3.70 ng	184181	1,4-Dichlorobenzene-d4			6.822

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2		000107-70-0	78
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2		000822-83-3	32
3	1-Propen-2-ol, acetate	100	C5H8O2		000108-22-5	12
4	2-Pentanone, 3-methyl-	100	C6H12O		000565-61-7	10
5	Acetamide, N-methyl-	73	C3H7NO		000079-16-3	9



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.228	2.5	ng	124550	1	6.822	996576	20.0
4-Penten-2-one,...	3.645	2.6	ng	130047	1	6.822	996576	20.0
3-Hexen-2-one	4.481	68.8	ng	3430760	1	6.822	996576	20.0
2-Pentanone, 4-...	5.087	82.0	ng	4088080	1	6.822	996576	20.0
2-Pentanone, 4-...	5.851	3.7	ng	184181	1	6.822	996576	20.0