

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102723\
 Data File : BF135979.D
 Acq On : 27 Oct 2023 12:16
 Operator : CG\JU
 Sample : PB156392BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB156392BL

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: BF135979.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	11	20	25	rVB	77429	111343	1.71%	0.249%
2	3.628	253	262	269	rVB	67032	95130	1.46%	0.213%
3	4.475	399	406	409	rBV	2271362	2740289	42.18%	6.130%
4	5.087	501	510	519	rBV	2176910	3681940	56.68%	8.237%
5	5.469	569	575	578	rBV	4720126	5555851	85.53%	12.429%
6	5.852	636	640	644	rBV	202130	159862	2.46%	0.358%
7	6.463	737	744	746	rBV	4339343	5457763	84.02%	12.210%
8	6.822	802	805	809	rVB	1079767	949738	14.62%	2.125%
9	7.393	895	902	905	rBV	3383660	3417756	52.61%	7.646%
10	8.104	1018	1023	1026	rBV	1637338	1262256	19.43%	2.824%
11	9.187	1201	1207	1210	rBV	6398693	5915981	91.07%	13.235%
12	9.863	1318	1322	1325	rVB	1770970	1373297	21.14%	3.072%
13	10.657	1452	1457	1460	rBV	4037576	3711084	57.13%	8.302%
14	11.351	1572	1575	1579	rBV	1616412	1408896	21.69%	3.152%
15	12.963	1843	1849	1852	rBV	5938619	6496007	100.00%	14.532%
16	14.010	2022	2027	2030	rBV	1347622	1257426	19.36%	2.813%
17	14.110	2039	2044	2050	rBV	64402	75497	1.16%	0.169%
18	15.498	2274	2280	2288	rBV	782232	1029770	15.85%	2.304%

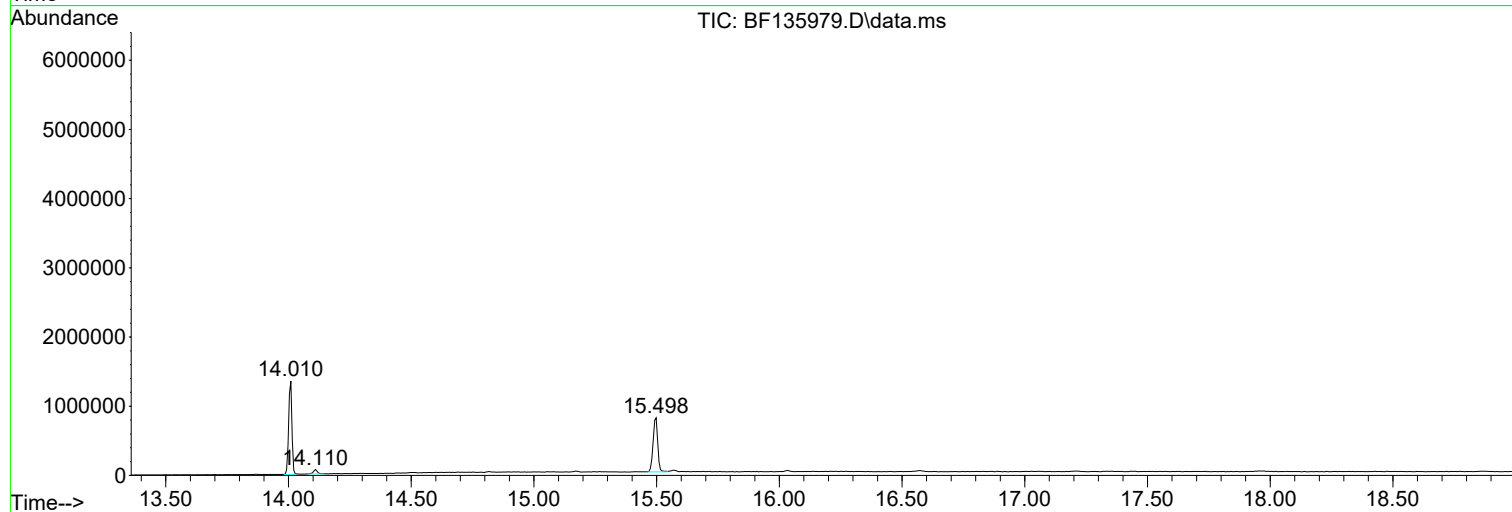
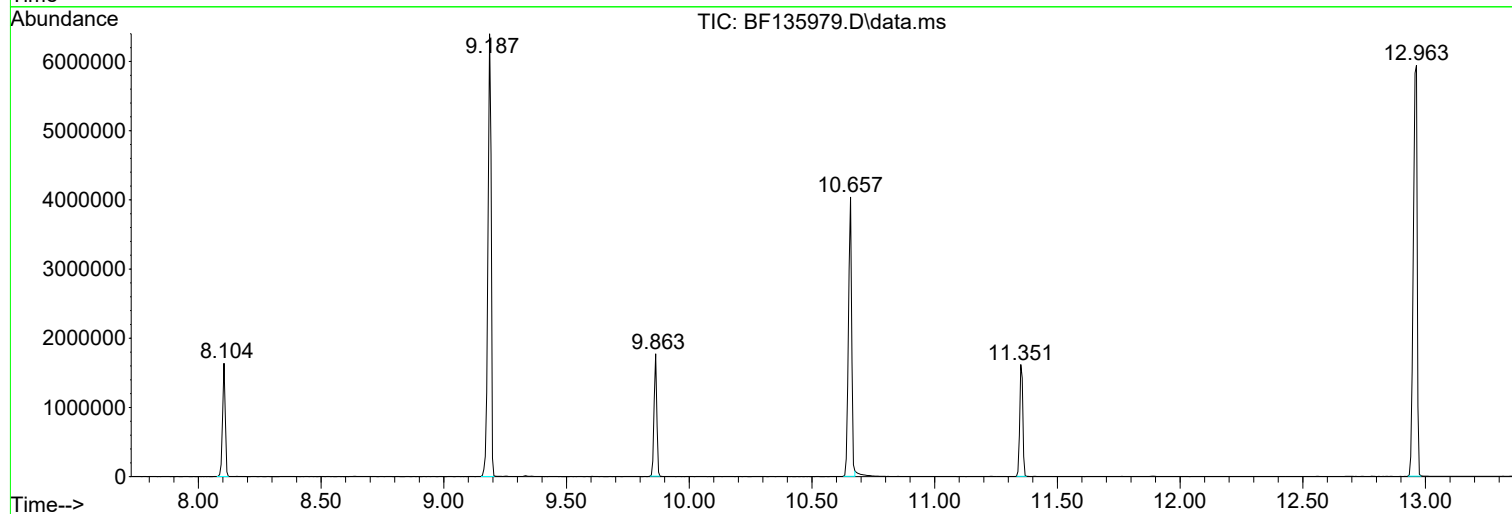
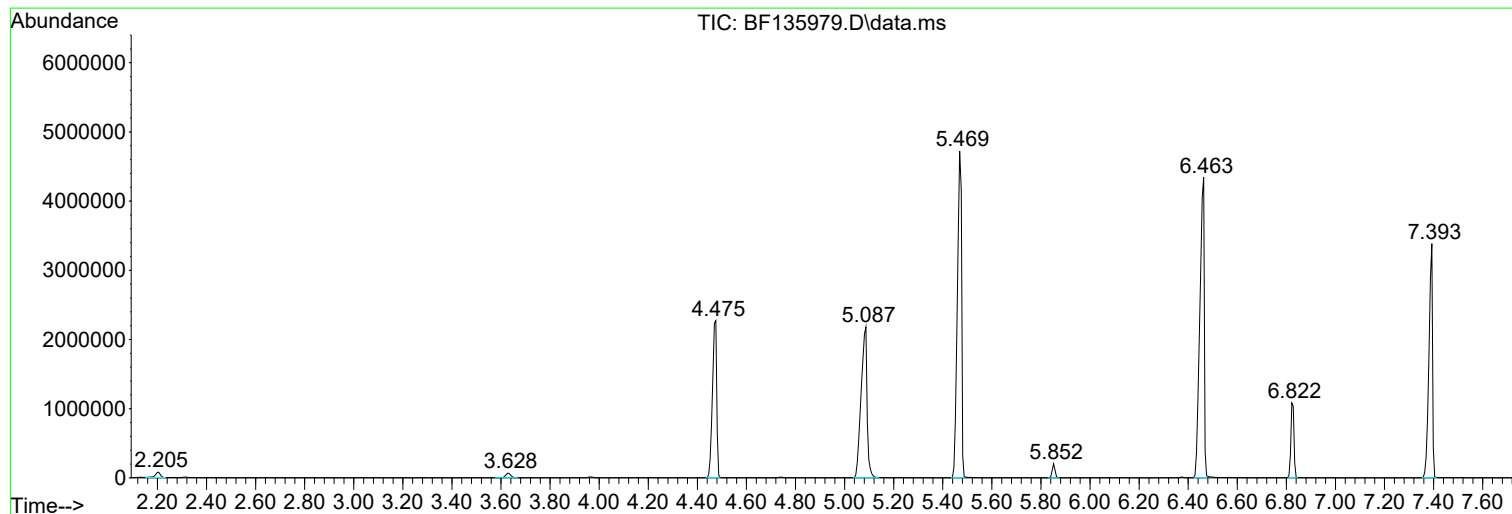
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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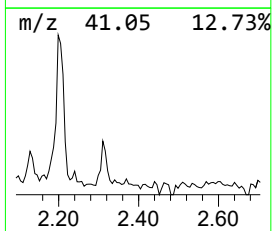
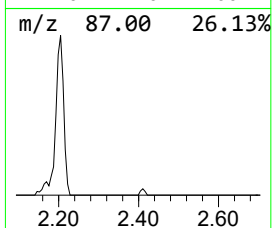
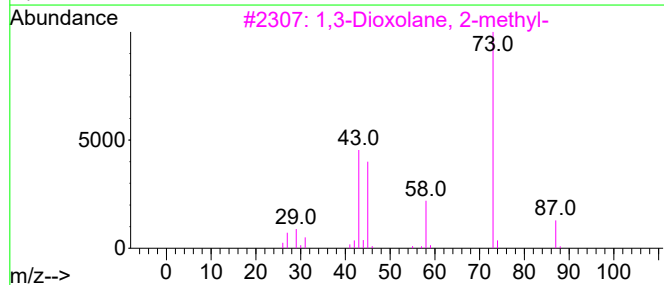
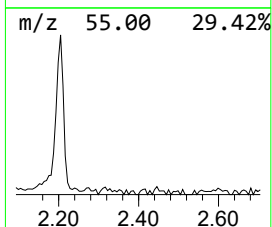
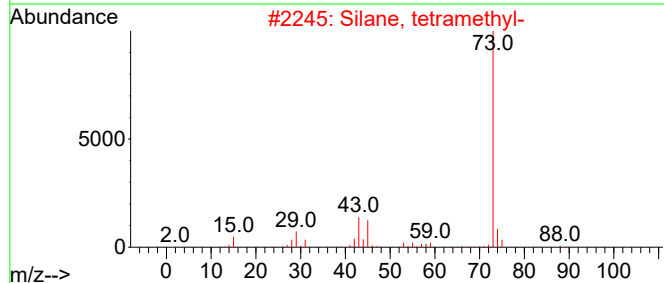
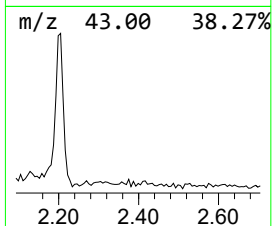
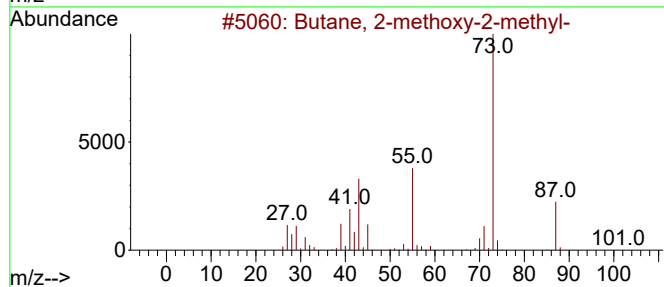
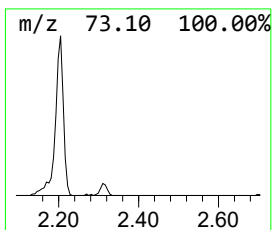
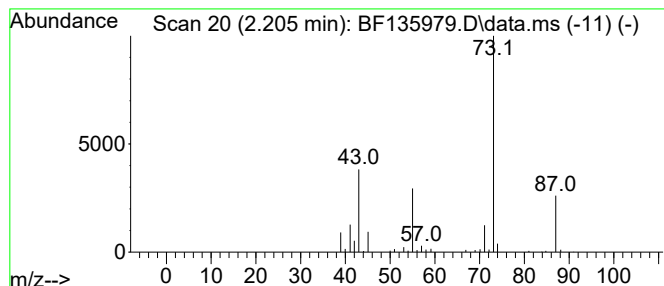
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	2.34 ng	111343	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9



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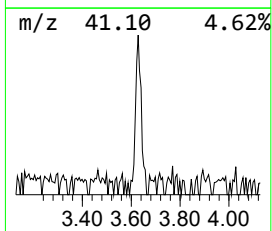
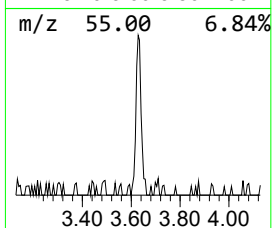
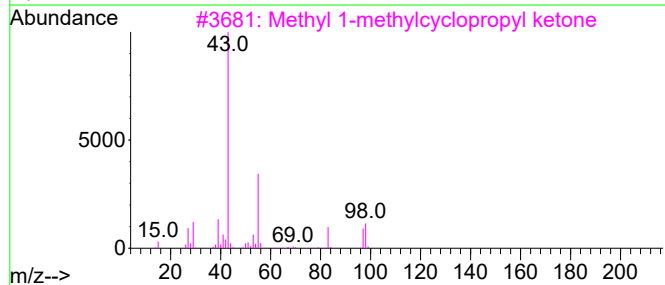
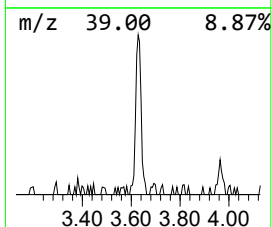
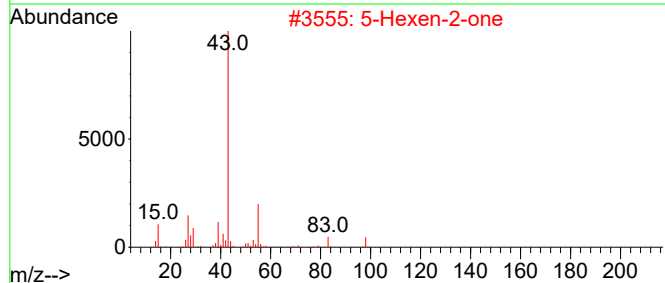
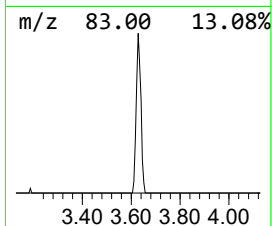
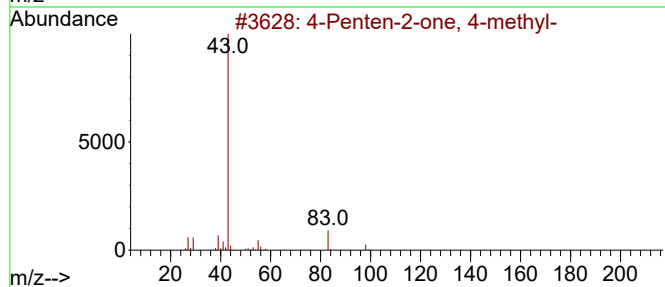
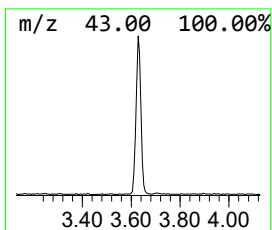
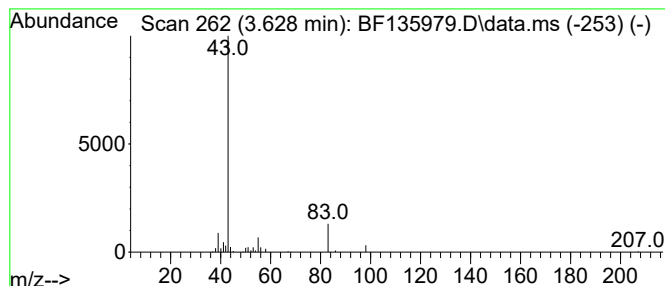
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.628	2.00 ng	95130	1,4-Dichlorobenzene-d4	6.828

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	22
3		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	12
4		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
5		2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	7



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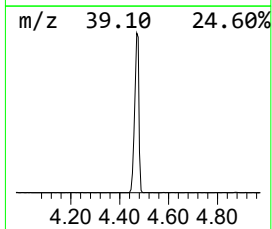
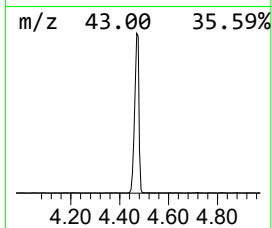
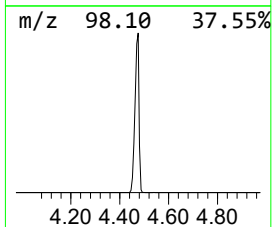
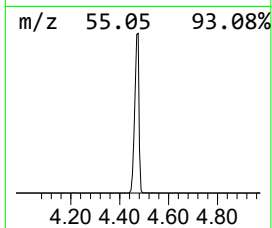
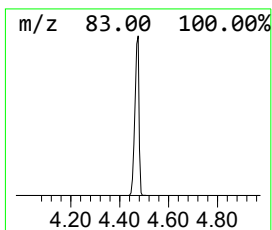
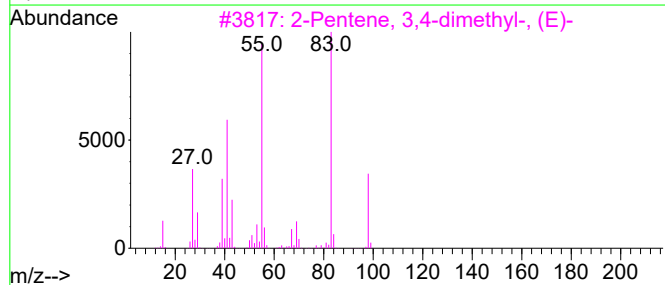
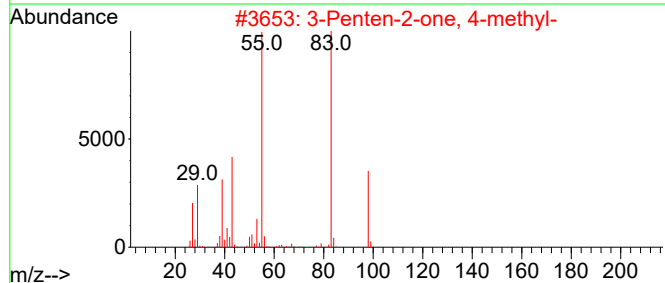
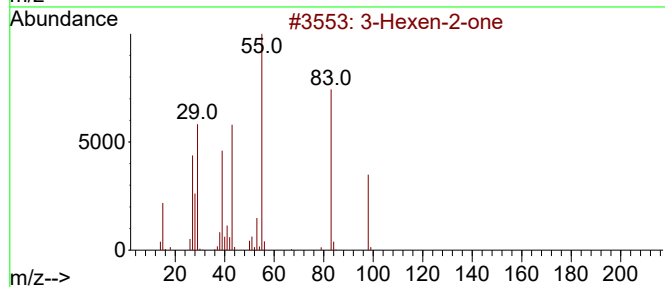
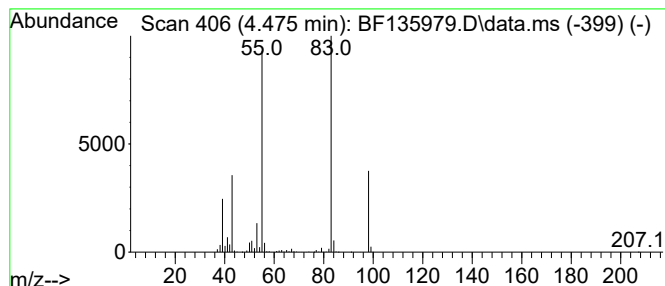
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.475	57.71 ng	2740290	1,4-Dichlorobenzene-d4	6.828

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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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB156392BL

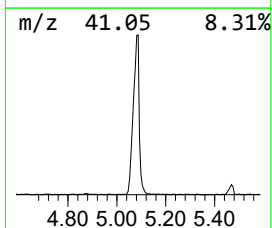
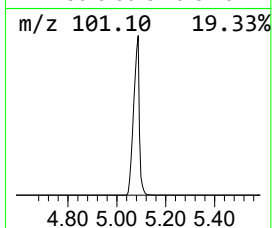
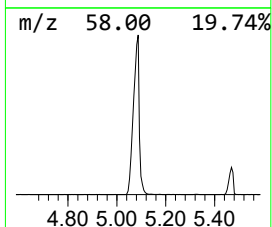
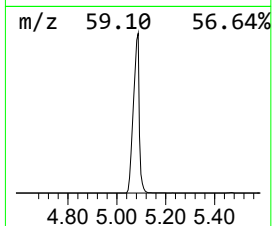
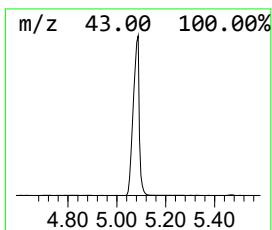
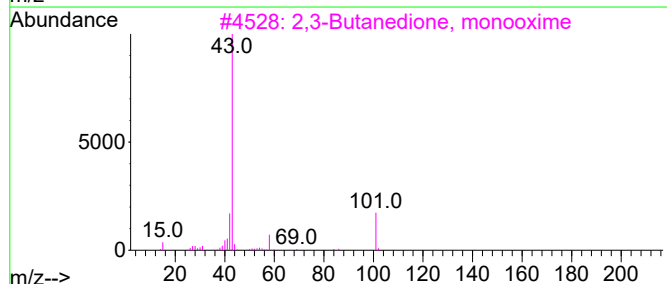
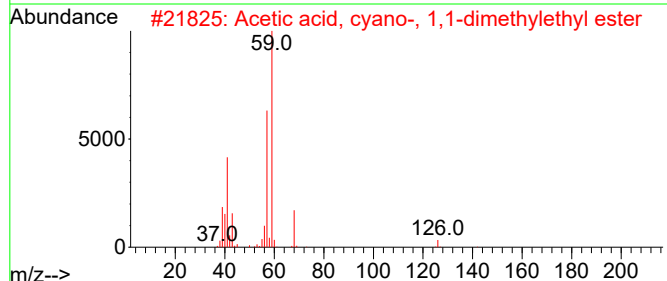
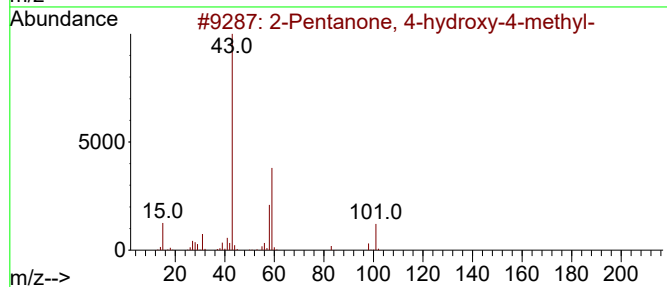
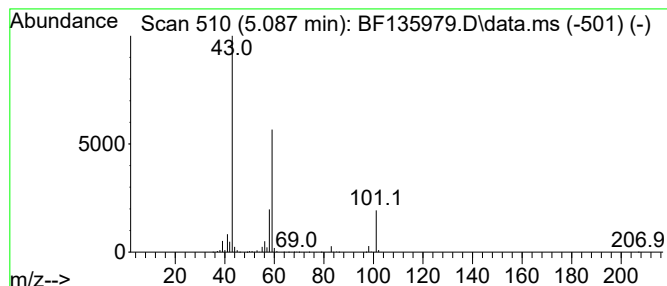
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	77.54 ng	3681940	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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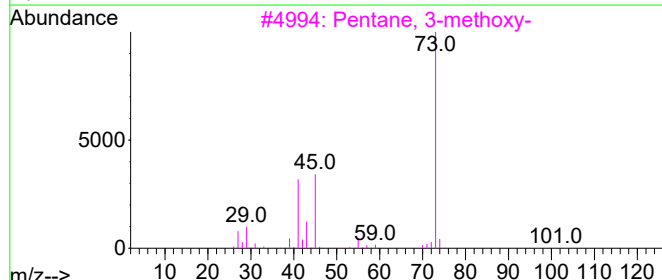
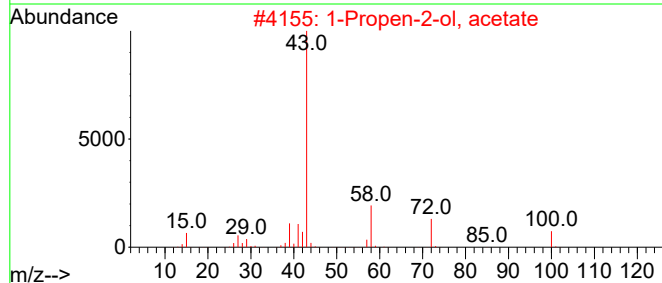
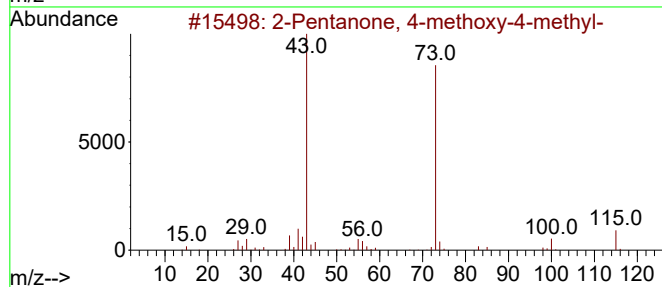
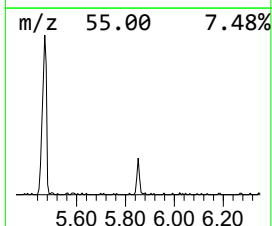
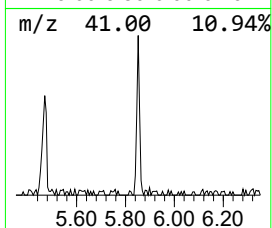
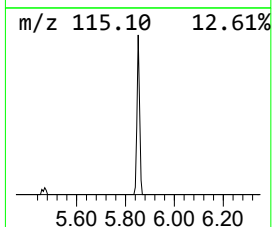
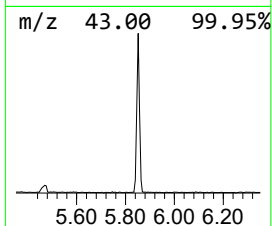
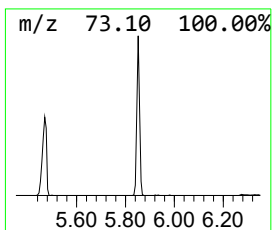
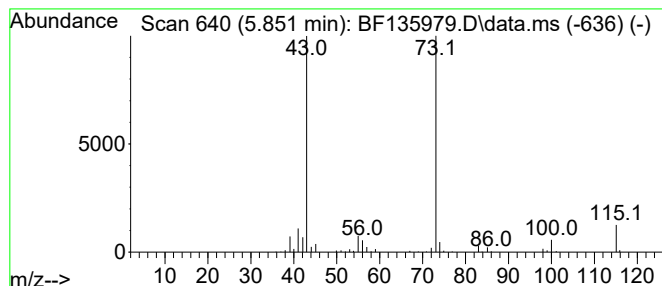
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	3.37 ng	159862	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
4			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10
5			N-Formylmorpholine	115	C5H9NO2	004394-85-8	10



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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...	2.205	2.3	ng	111343	1	6.828	949738	20.0
4-Penten-2-one,...	3.628	2.0	ng	95130	1	6.828	949738	20.0
3-Hexen-2-one	4.475	57.7	ng	2740290	1	6.828	949738	20.0
2-Pentanone, 4-...	5.087	77.5	ng	3681940	1	6.828	949738	20.0
2-Pentanone, 4-...	5.851	3.4	ng	159862	1	6.828	949738	20.0