

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100322\
 Data File : BM036823.D
 Acq On : 03 Oct 2022 18:49
 Operator : CG/JU
 Sample : PB148034BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB148034BL

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_M\Methods\8270-BM100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036823.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.834	122	127	132	rBV	234401	278329	1.21%	0.219%
2	4.451	227	232	242	rBV	2618727	3373504	14.66%	2.651%
3	5.075	330	338	351	rBV	7108532	10427715	45.33%	8.193%
4	5.534	409	416	432	rBV	9369290	13052581	56.74%	10.255%
5	6.157	516	522	531	rVB	515888	758917	3.30%	0.596%
6	7.139	680	689	703	rBV	8776039	13592445	59.08%	10.679%
7	7.975	824	831	839	rBV	1541721	2390524	10.39%	1.878%
8	9.145	1021	1030	1045	rBV	4983104	8291232	36.04%	6.514%
9	10.780	1296	1308	1325	rBV	2079233	3495502	15.19%	2.746%
10	13.233	1717	1725	1738	rBV	13125970	18800075	81.72%	14.771%
11	14.598	1951	1957	1969	rBV	3029015	4477011	19.46%	3.518%
12	16.086	2202	2210	2230	rBV	9111438	13075569	56.84%	10.273%
13	17.339	2416	2423	2436	rBV	3648281	5091625	22.13%	4.000%
14	19.950	2862	2867	2877	rBV	17917133	23005202	100.00%	18.075%
15	21.503	3126	3131	3141	rBV	3209305	4189026	18.21%	3.291%
16	23.915	3535	3541	3554	rVB2	1452315	2978229	12.95%	2.340%

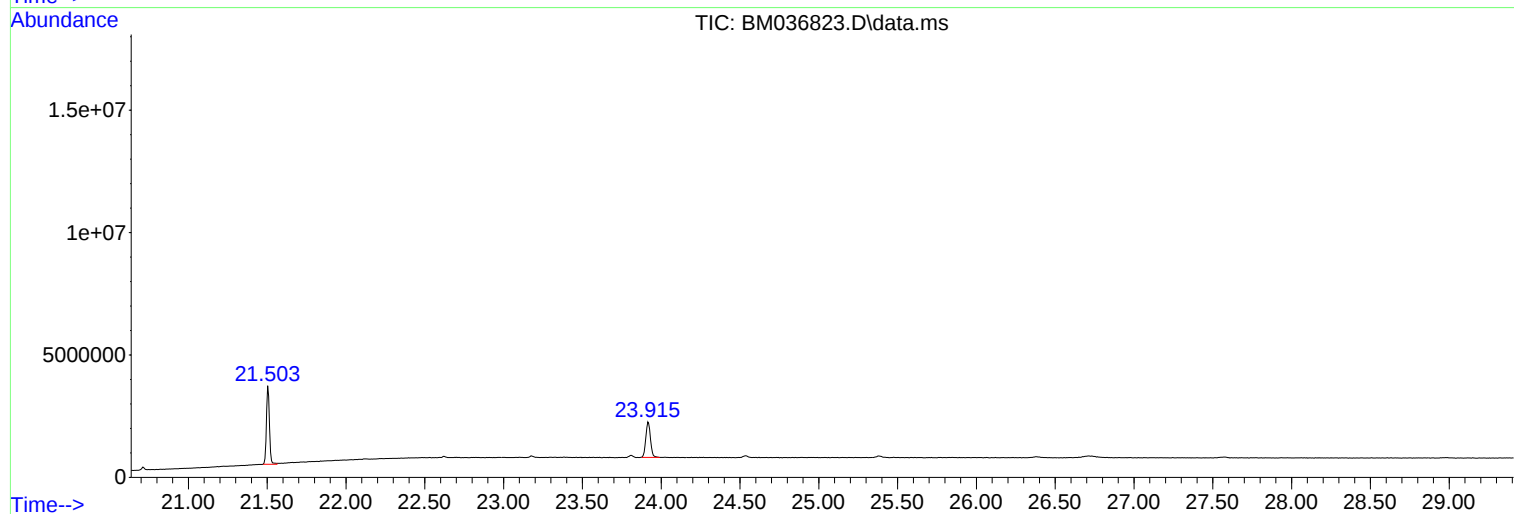
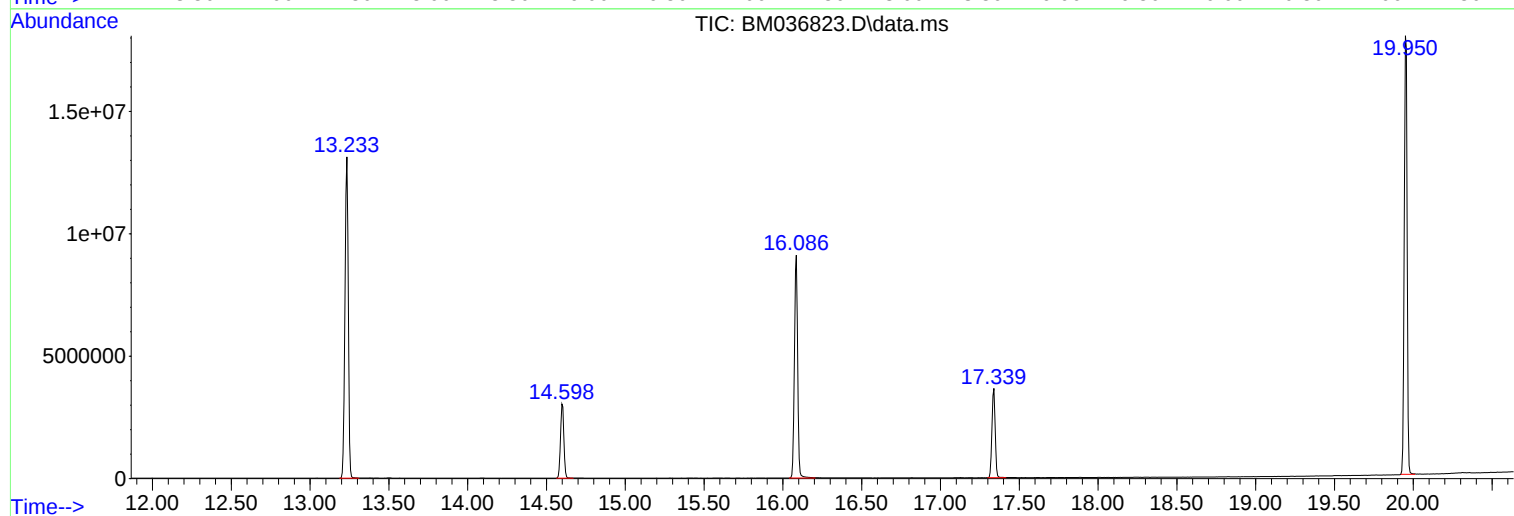
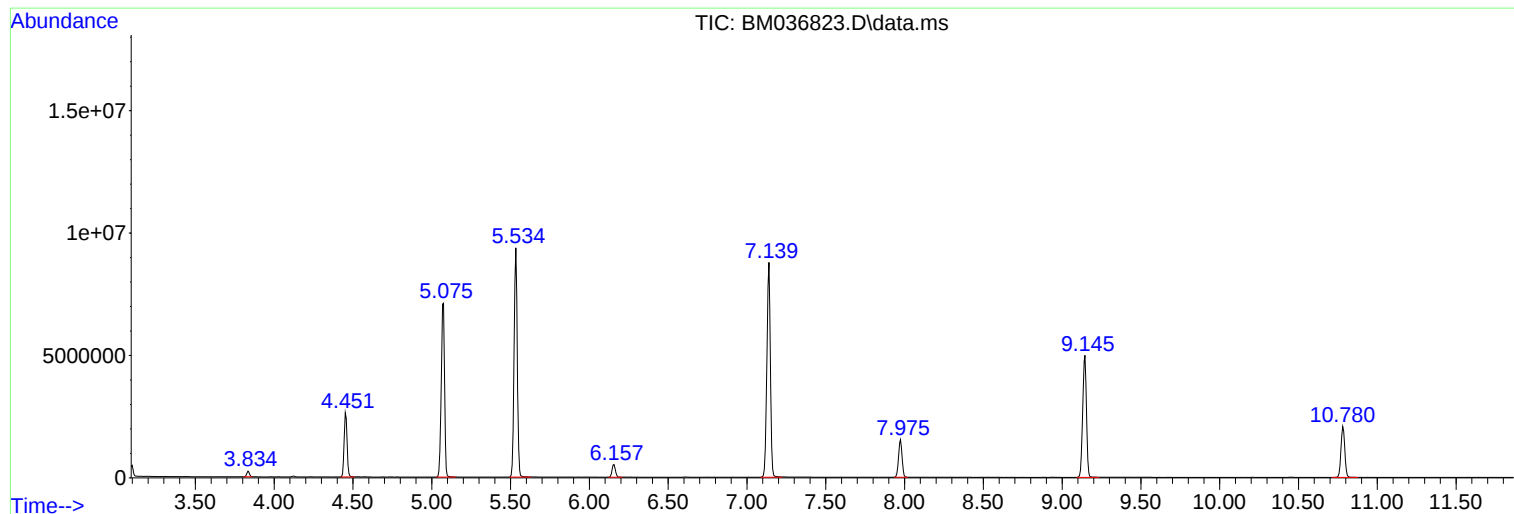
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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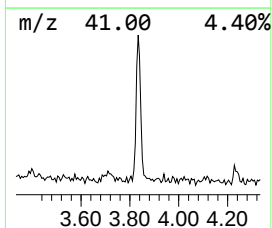
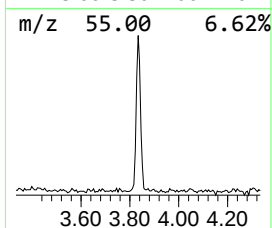
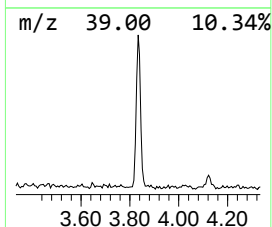
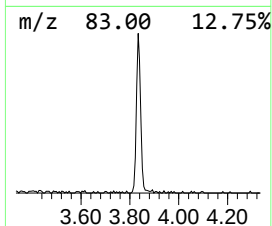
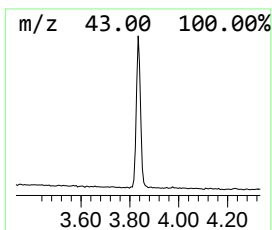
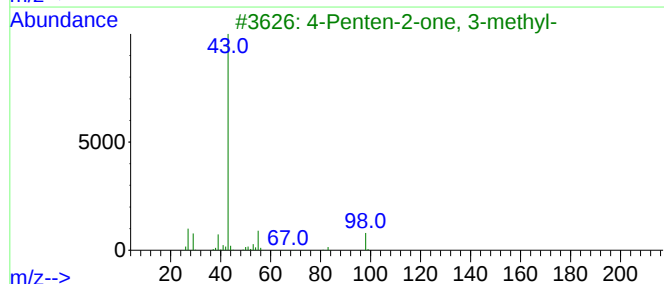
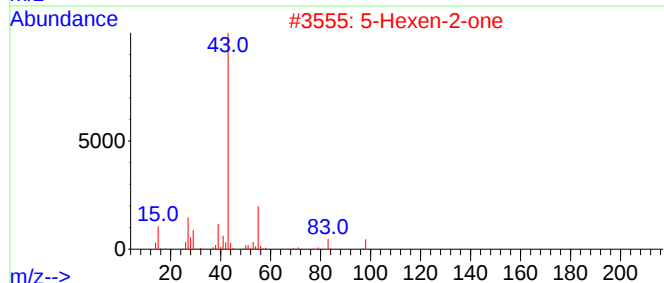
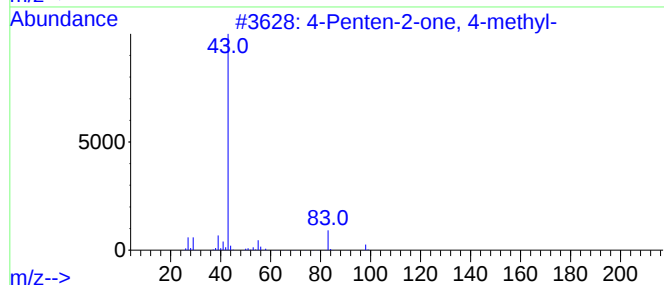
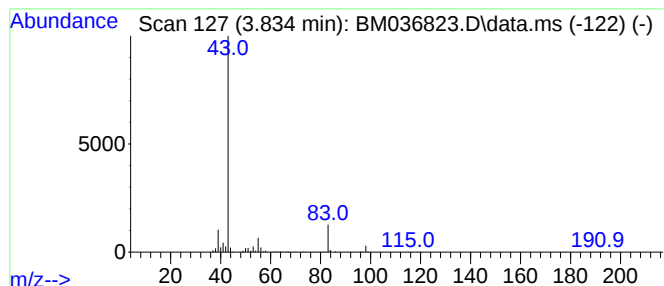
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.834	2.33 ng	278329	1,4-Dichlorobenzene-d4	7.975

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	47
3			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	43
4			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	12
5			4-Hexen-2-one	98	C6H10O	025659-22-7	9



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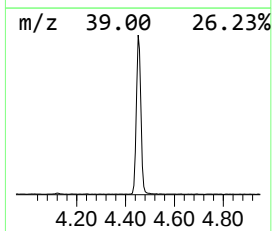
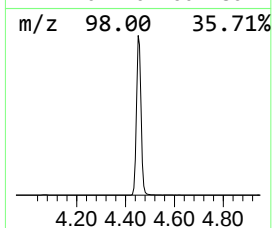
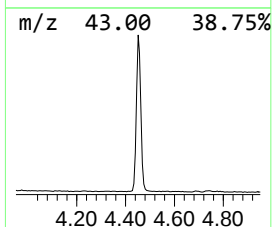
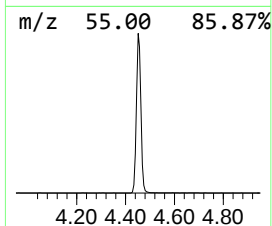
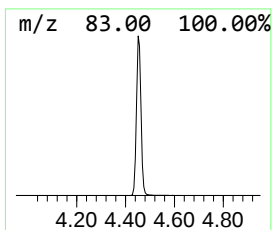
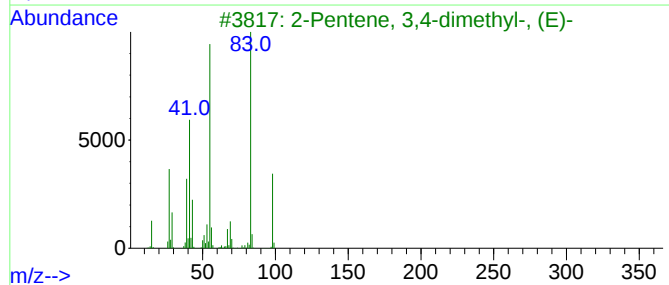
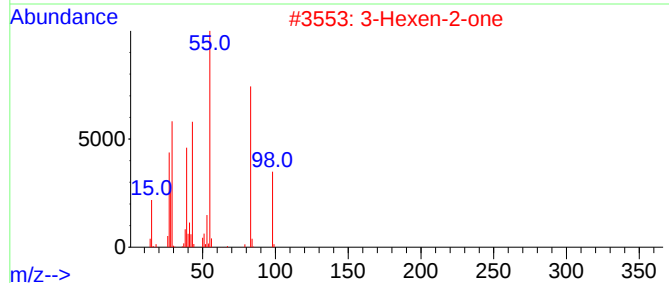
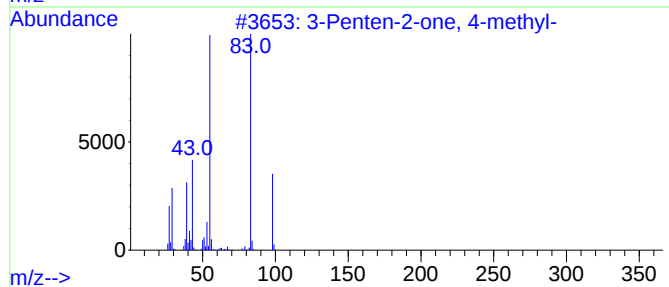
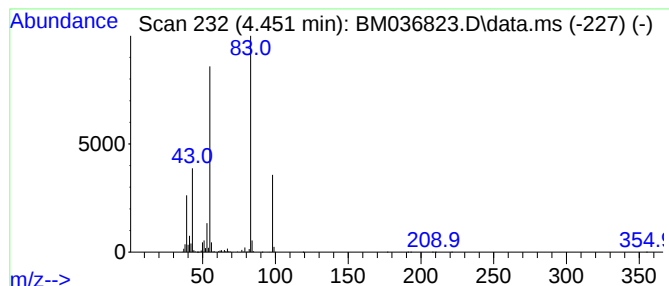
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.451	28.22 ng	3373500	1,4-Dichlorobenzene-d4	7.975

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-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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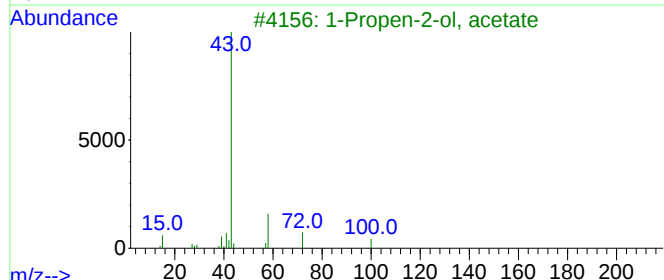
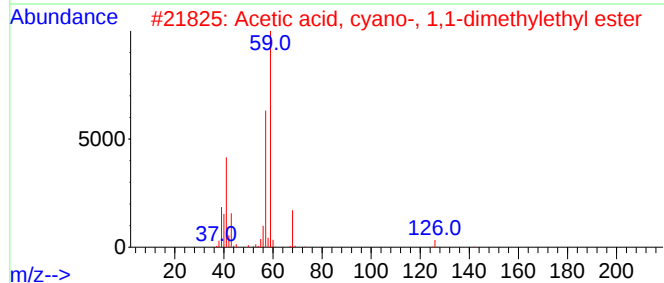
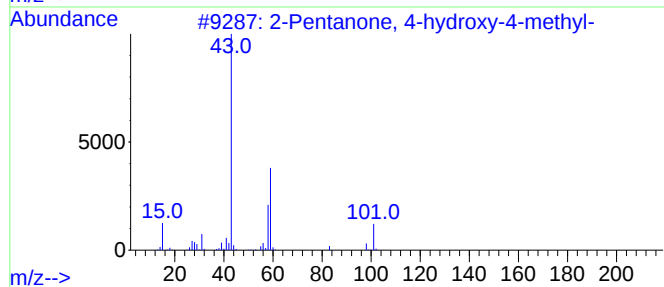
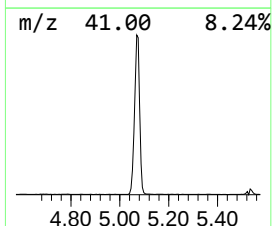
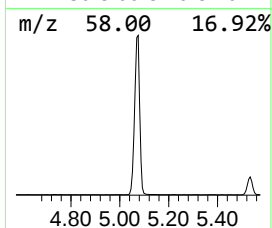
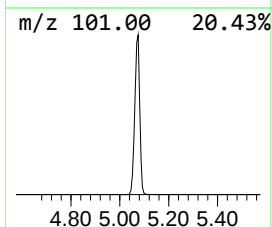
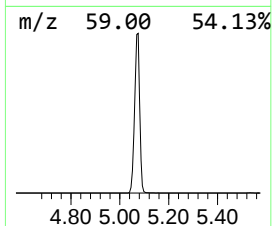
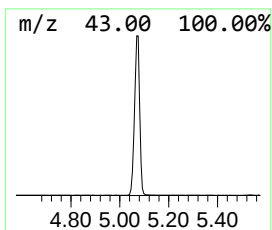
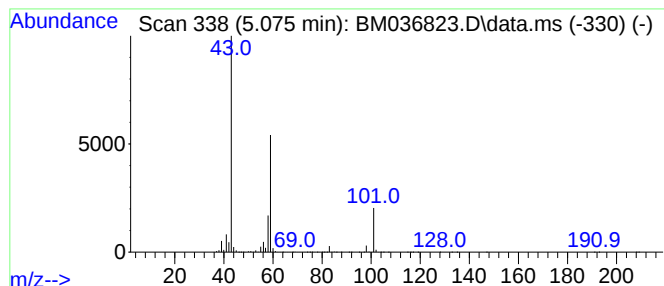
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	87.24 ng	10427700	1,4-Dichlorobenzene-d4	7.975

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	17
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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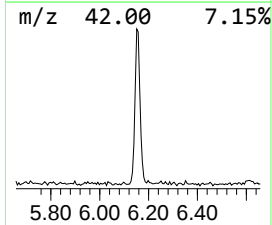
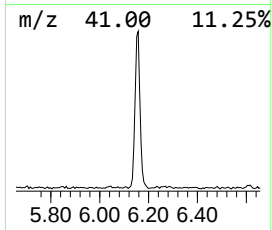
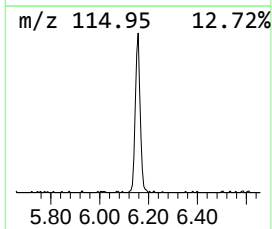
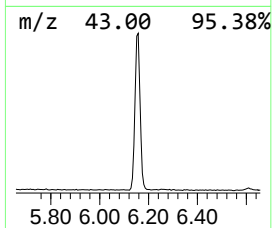
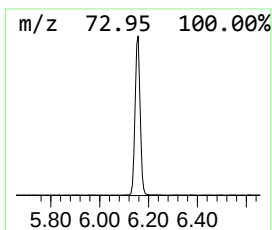
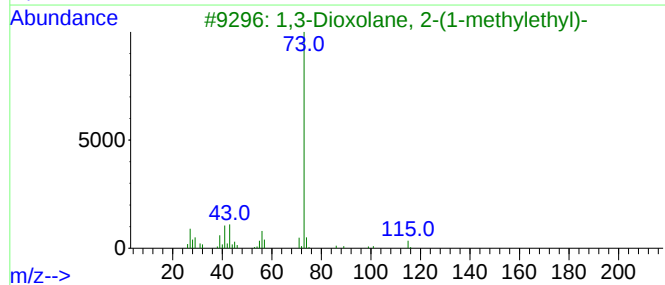
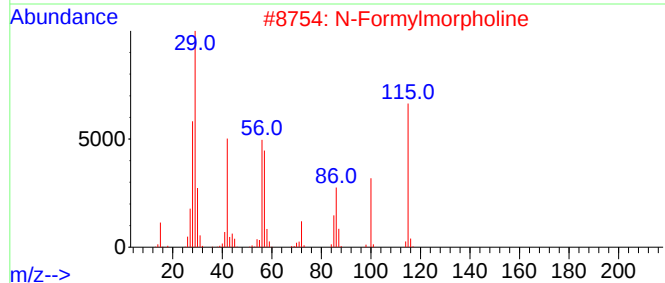
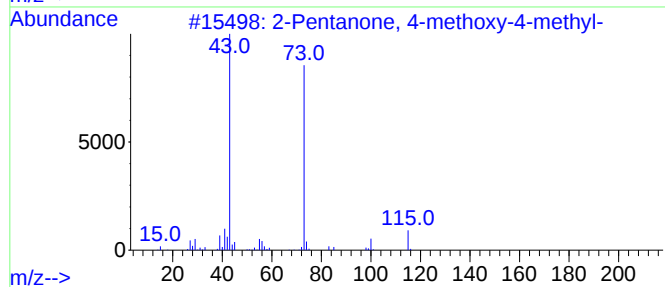
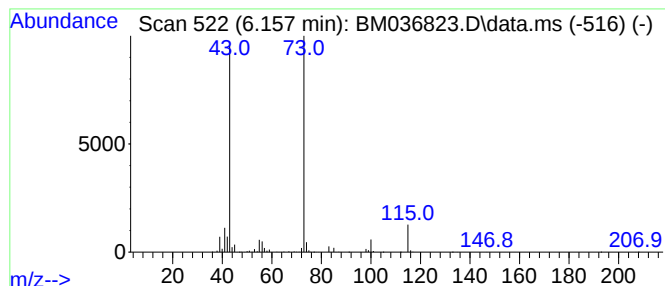
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.157	6.35 ng	758917	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83		
2	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10		
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10		
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9		
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one,...	3.834	2.3	ng	278329	1	7.975	2390520	20.0
3-Penten-2-one,...	4.451	28.2	ng	3373500	1	7.975	2390520	20.0
2-Pentanone, 4-...	5.075	87.2	ng	10427700	1	7.975	2390520	20.0
2-Pentanone, 4-...	6.157	6.3	ng	758917	1	7.975	2390520	20.0