

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
 Data File : BF101475.D
 Acq On : 18 Dec 2017 12:48
 Operator : SJ/JU
 Sample : PB105093BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB105093BL

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.528	240	245	265	rBV	441442	790078	16.56%	1.866%
2	4.410	390	395	414	rBV	1846286	2364822	49.56%	5.586%
3	5.040	497	502	524	rBV	1010078	1679051	35.19%	3.966%
4	5.440	565	570	595	rBV	3473313	4088961	85.69%	9.658%
5	6.451	737	742	759	rBV	3208359	4046819	84.81%	9.559%
6	6.581	759	764	767	rBV	3801770	3808965	79.82%	8.997%
7	6.804	799	802	811	rBV	1066900	954342	20.00%	2.254%
8	6.963	824	829	838	rBV	3100747	3181832	66.68%	7.516%
9	7.375	894	899	917	rBV	2486257	2741420	57.45%	6.475%
10	8.087	1016	1020	1035	rBV	1273393	1276053	26.74%	3.014%
11	9.163	1197	1203	1206	rBV	4279990	4596414	96.33%	10.857%
12	9.792	1302	1310	1314	rBV2	59333	105222	2.21%	0.249%
13	9.845	1314	1319	1329	rVB	1408745	1428632	29.94%	3.375%
14	10.639	1450	1454	1468	rBV	2575336	2706351	56.72%	6.393%
15	11.333	1568	1572	1581	rBV	1468101	1580899	33.13%	3.734%
16	12.922	1837	1842	1845	rBV	4207007	4771751	100.00%	11.271%
17	13.986	2019	2023	2033	rBV	1333784	1452781	30.45%	3.432%
18	15.457	2268	2273	2287	rVB2	482177	761613	15.96%	1.799%

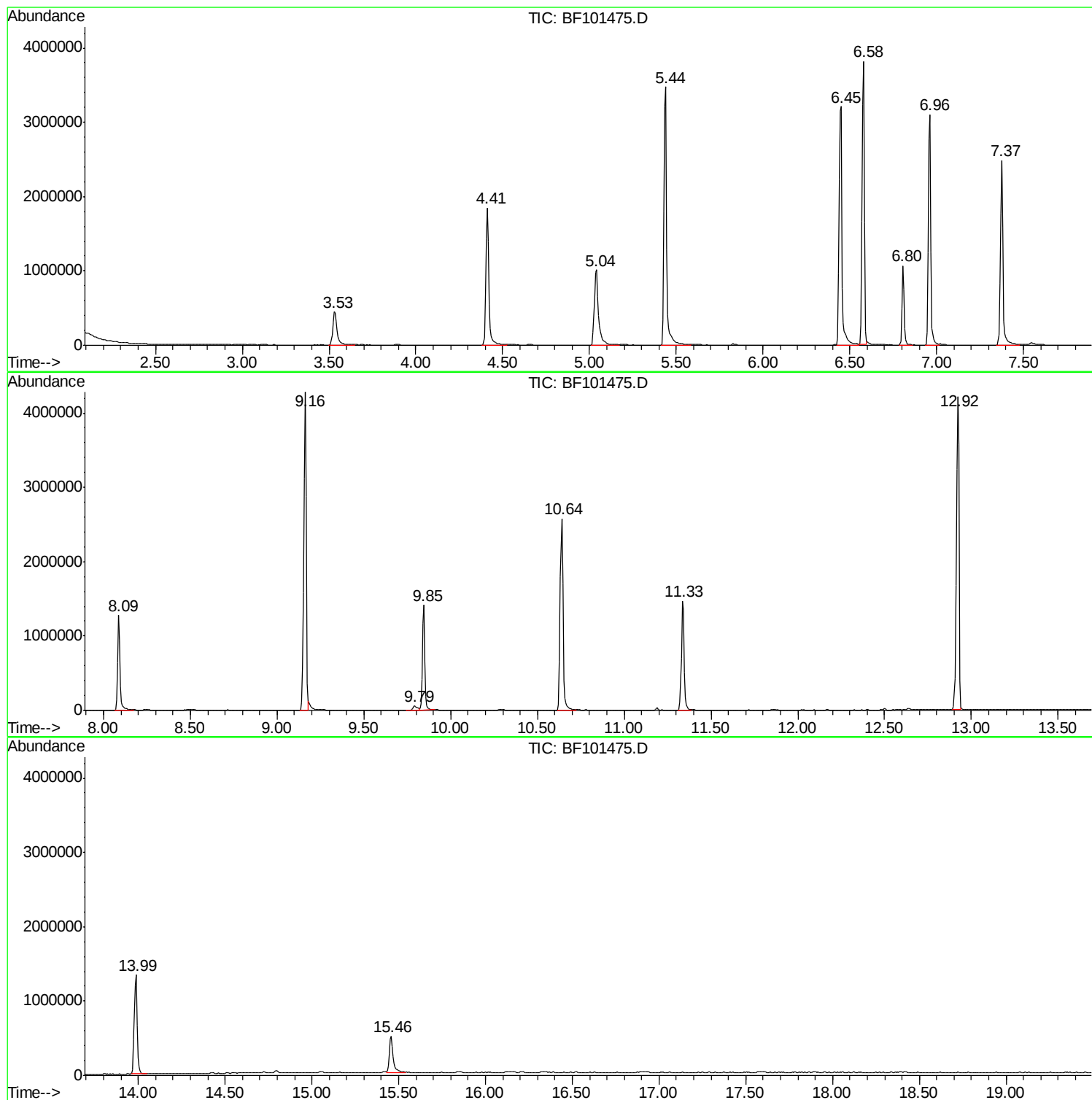
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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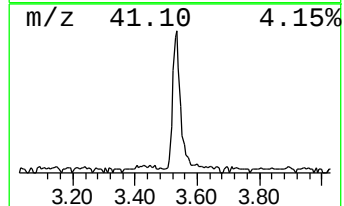
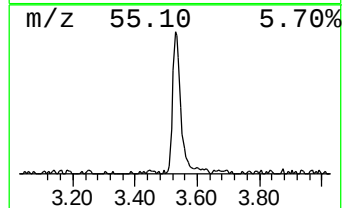
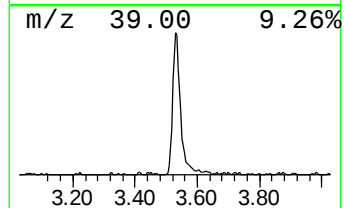
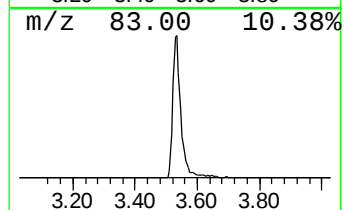
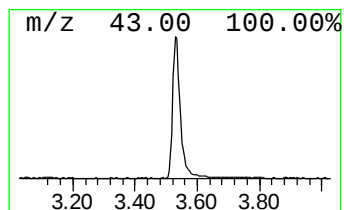
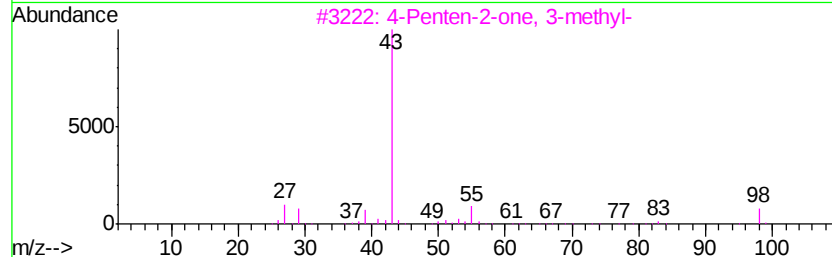
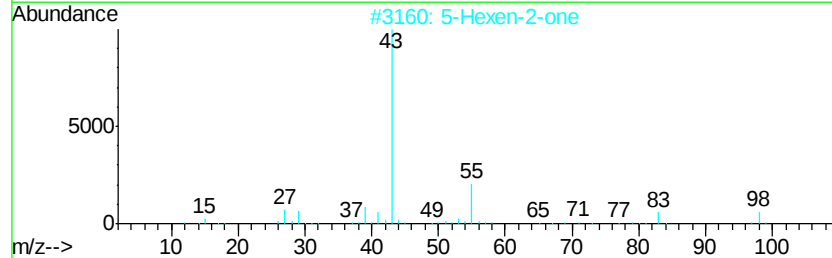
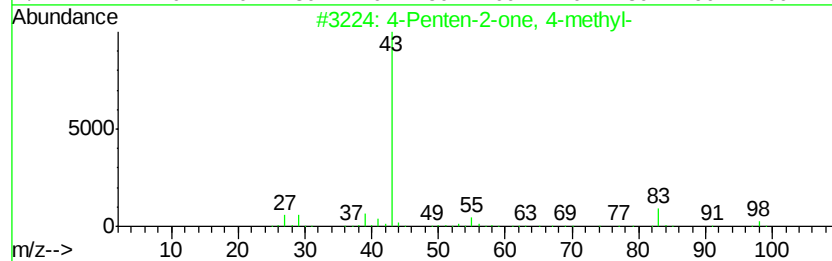
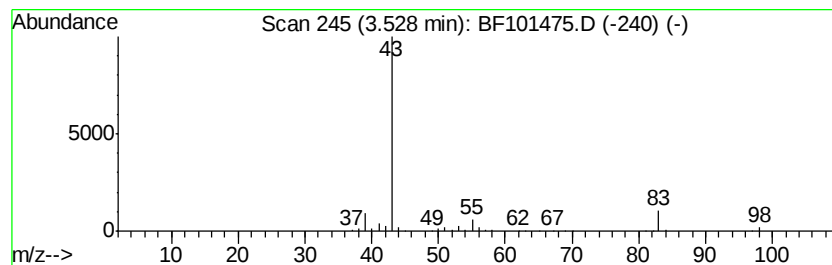
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	16.56 ng	790078	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2		5-Hexen-2-one	98	C6H10O	000109-49-9	40
3		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	36
4		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	16
5		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9



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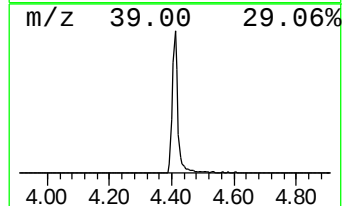
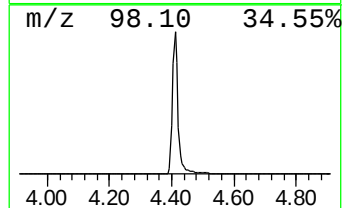
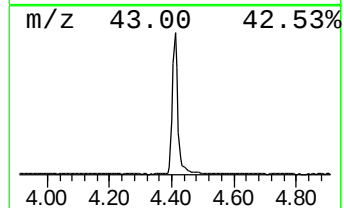
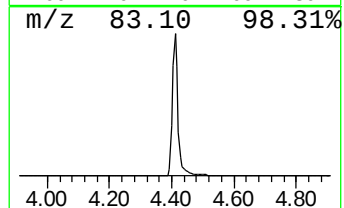
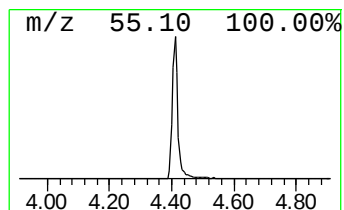
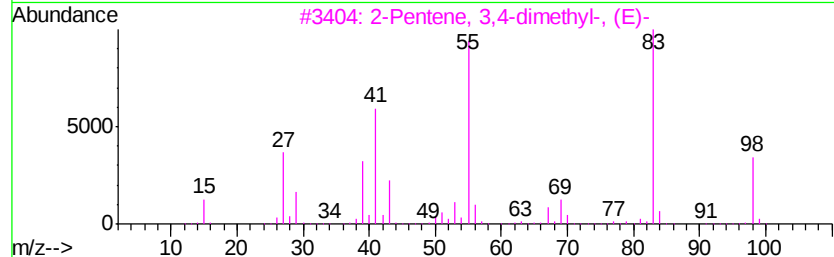
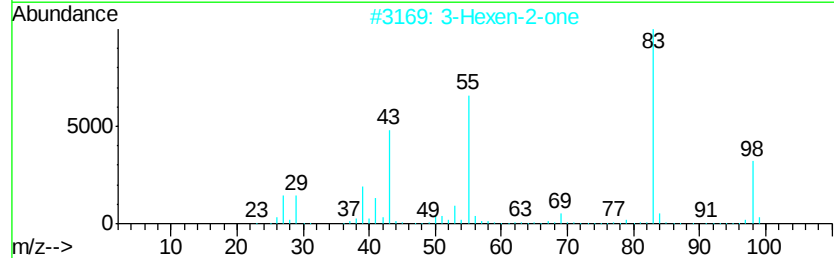
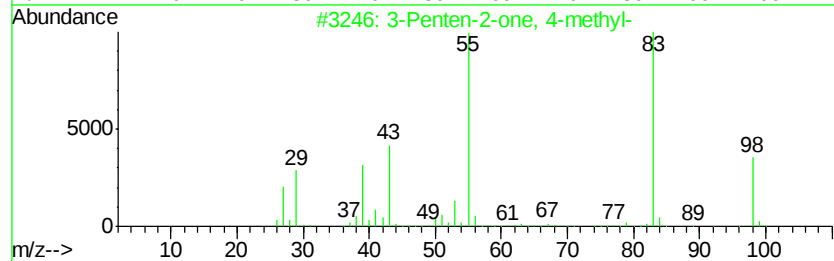
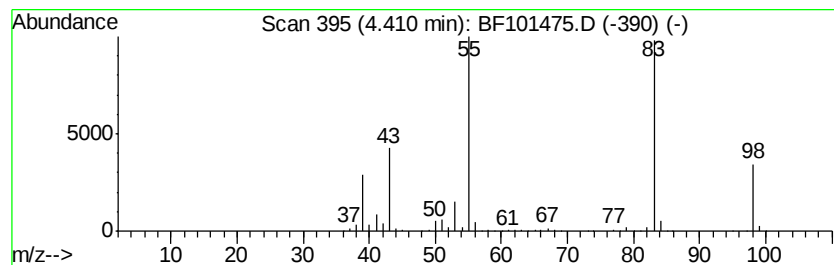
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	49.56 ng	2364820	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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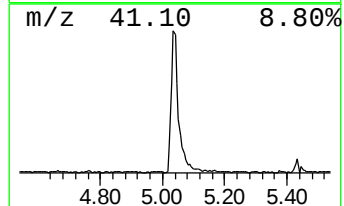
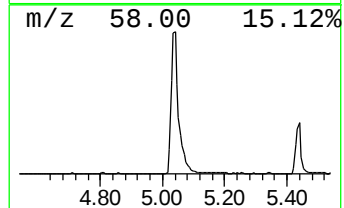
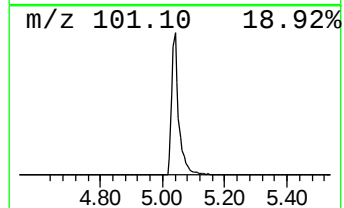
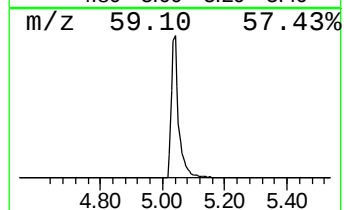
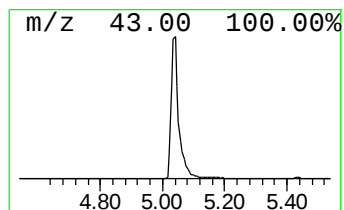
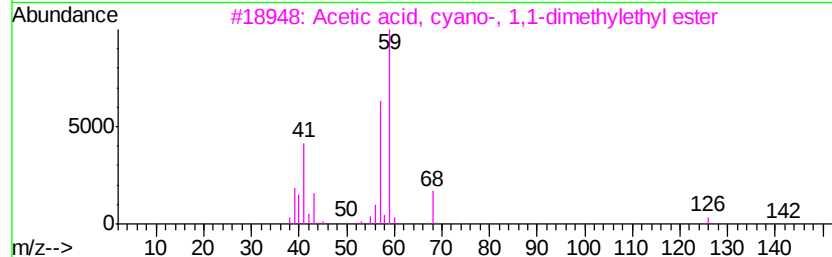
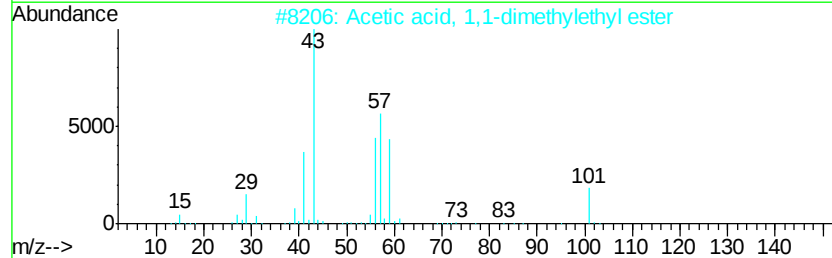
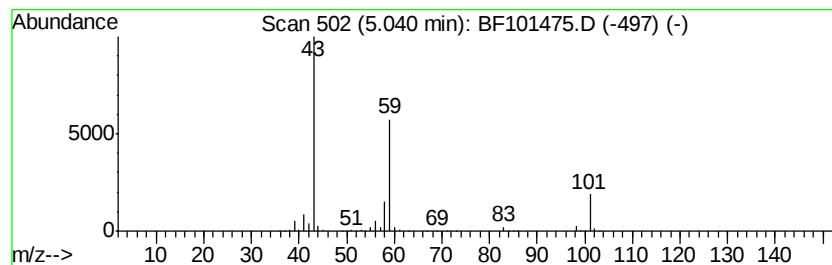
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	35.19 ng	1679050	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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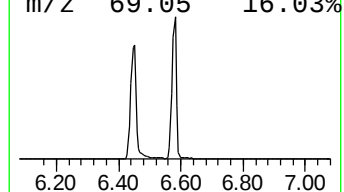
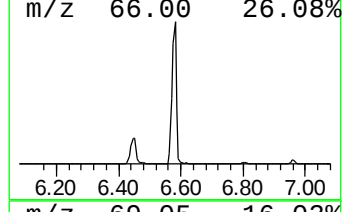
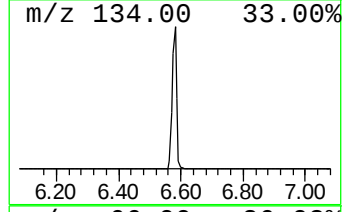
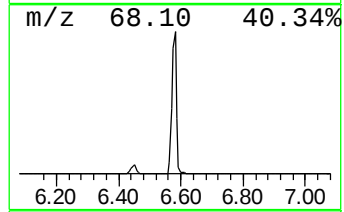
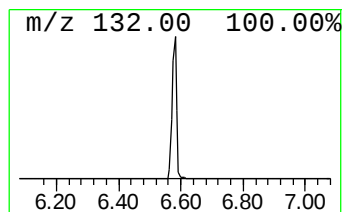
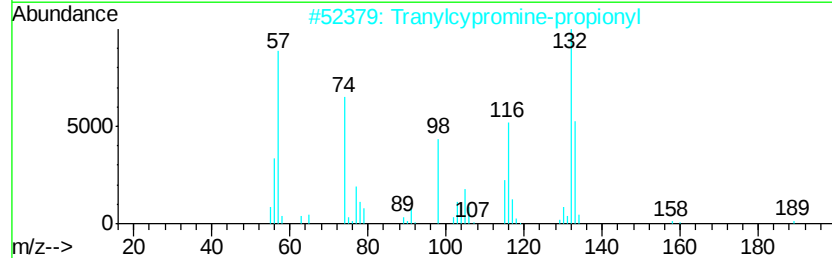
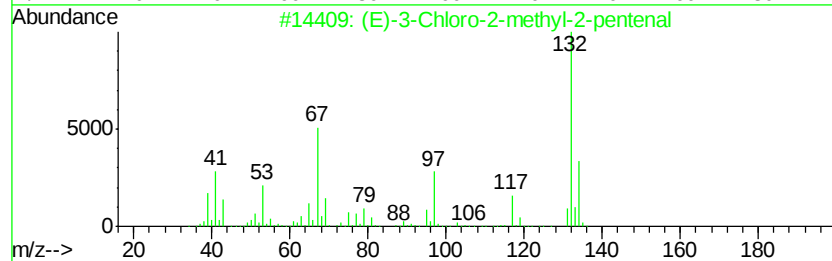
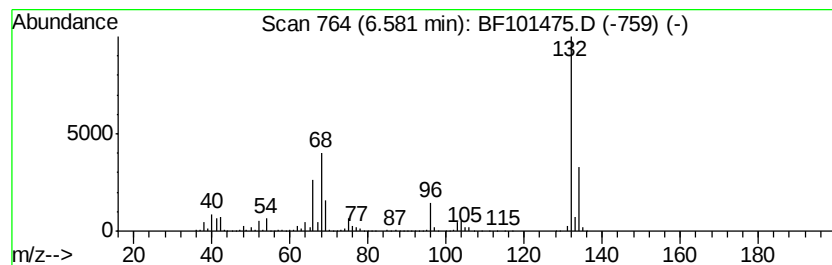
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Peak Number 4 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	79.82 ng	3808970	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	3.53	16.6	ng	790078	1	6.80	954342	20.0
3-Penten-2-one, 4...	4.41	49.6	ng	2364820	1	6.80	954342	20.0
2-Pentanone, 4-hy...	5.04	35.2	ng	1679050	1	6.80	954342	20.0
unknown6.58	6.58	79.8	ng	3808970	1	6.80	954342	20.0