

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061022\
 Data File : BG053882.D
 Acq On : 10 Jun 2022 19:36
 Operator : CG/JU
 Sample : N3299-06
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SC-18

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_G\Methods\8270-BG060222.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053882.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.975	95	100	109	rVB	70946	112056	2.25%	1.032%
2	4.598	197	206	223	rVB	2866467	4974664	100.00%	45.826%
3	5.191	299	307	319	rVB	729255	1238129	24.89%	11.406%
4	8.088	794	800	807	rVB	56158	97138	1.95%	0.895%
5	8.728	903	909	918	rBV	48739	89787	1.80%	0.827%
6	9.245	990	997	1006	rBV	147920	273351	5.49%	2.518%
7	10.896	1270	1278	1287	rBV	71944	133467	2.68%	1.229%
8	13.335	1686	1693	1701	rBV	450107	736194	14.80%	6.782%
9	14.710	1921	1927	1935	rVB	128563	205964	4.14%	1.897%
10	17.453	2387	2394	2406	rBV	196337	306926	6.17%	2.827%
11	20.062	2832	2838	2850	rVB	1277292	1748898	35.16%	16.111%
12	21.372	3056	3061	3072	rBV3	33260	59315	1.19%	0.546%
13	21.731	3115	3122	3129	rBV2	255499	435820	8.76%	4.015%
14	24.998	3667	3678	3689	rBV2	148161	443804	8.92%	4.088%

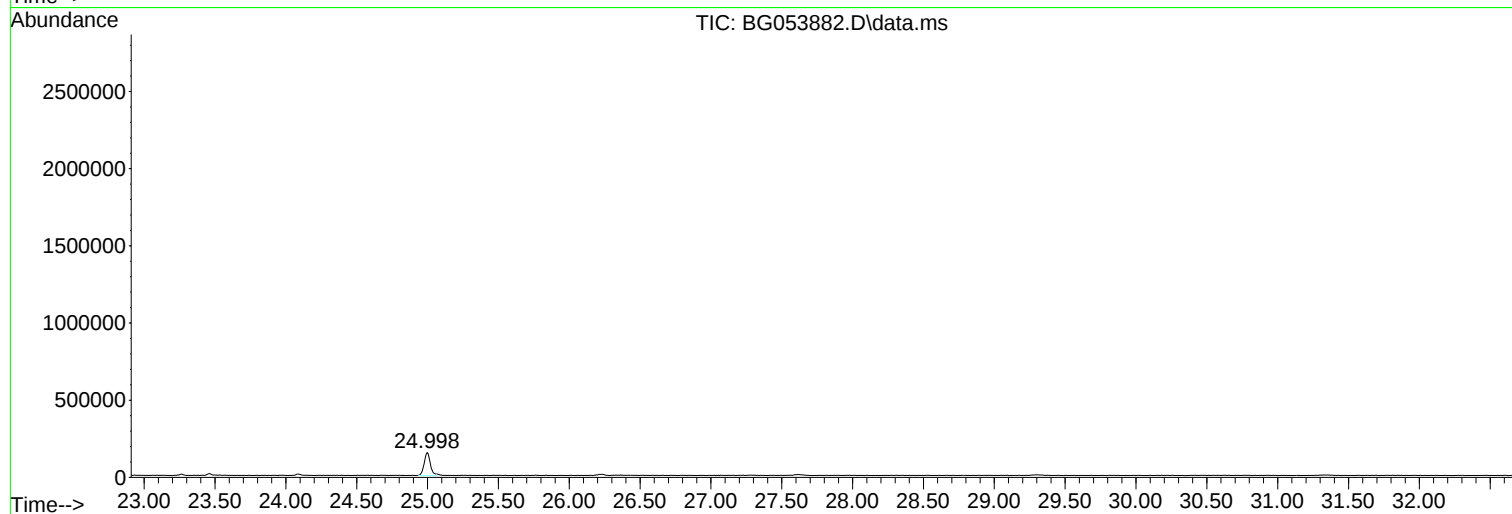
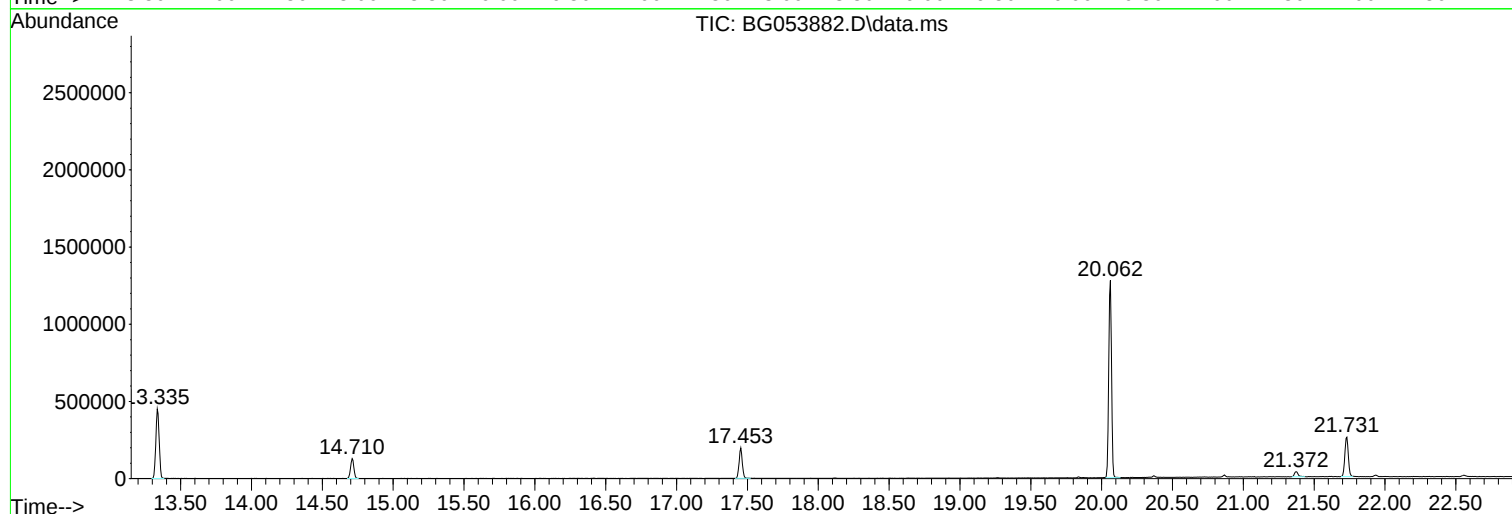
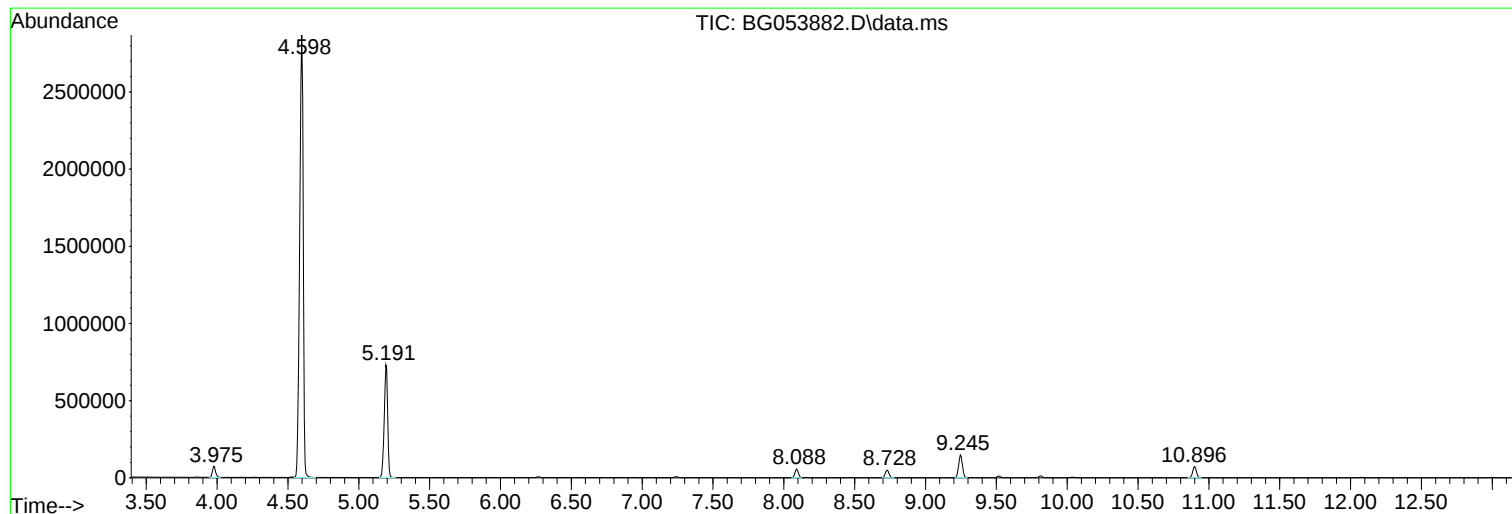
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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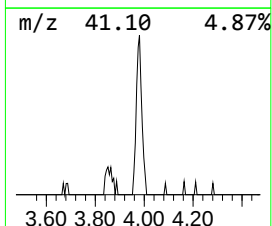
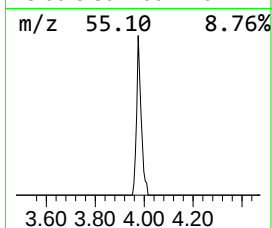
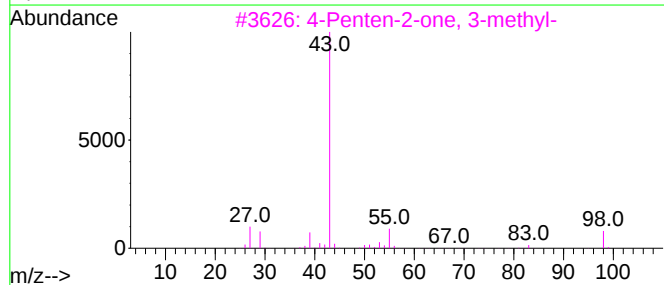
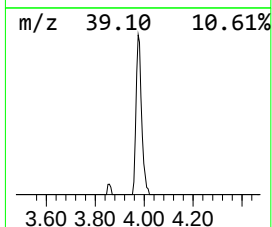
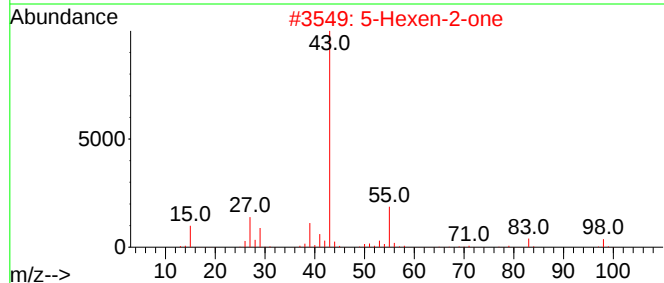
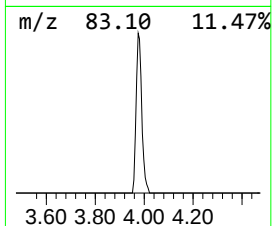
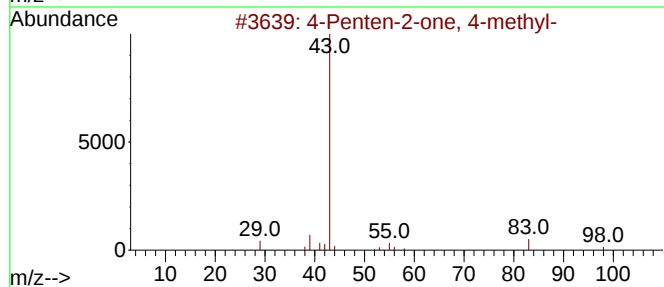
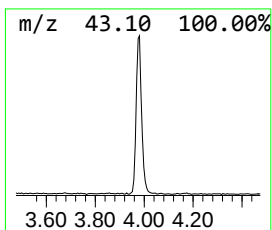
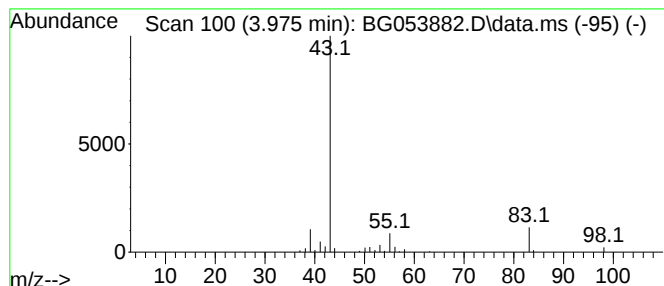
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.975 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.975	23.07 ng	112056	1,4-Dichlorobenzene-d4	8.088

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	53
2		5-Hexen-2-one	98	C6H10O	000109-49-9	52
3		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	36
4		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17
5		Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	12



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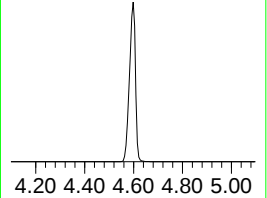
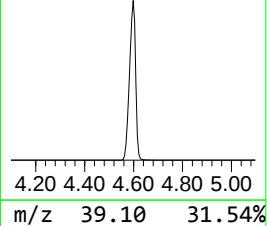
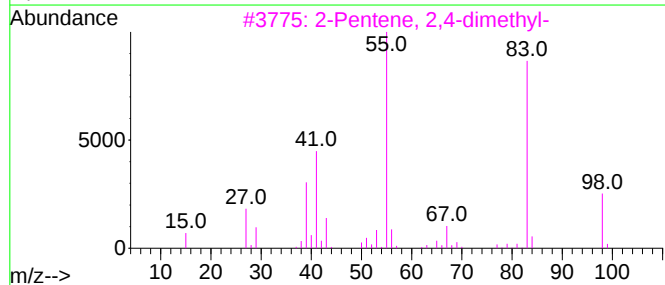
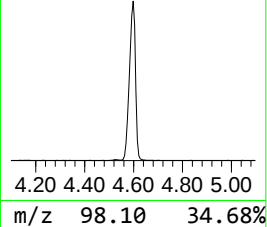
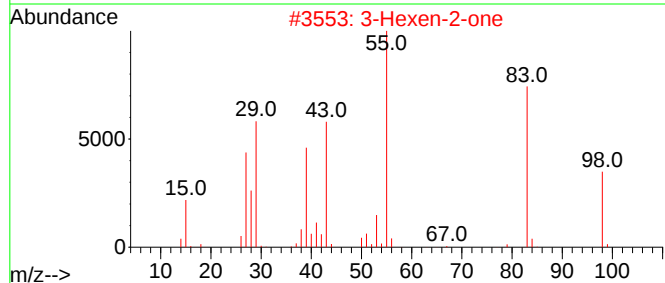
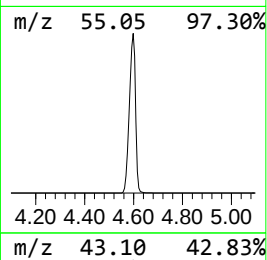
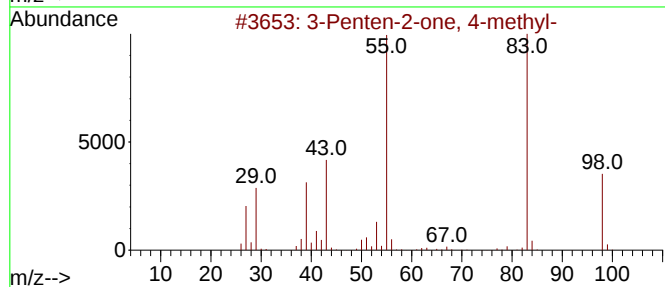
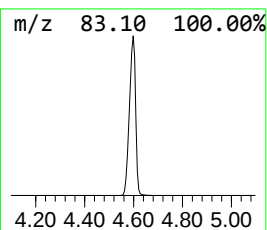
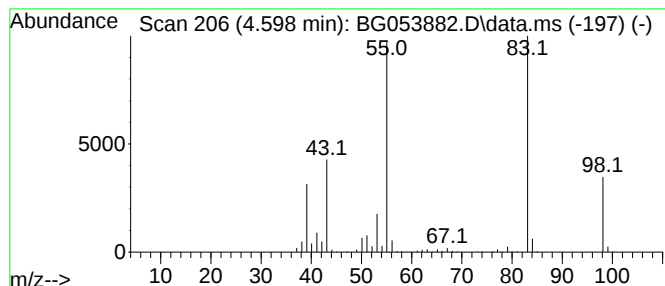
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.598	1024.25 ng	4974660	1,4-Dichlorobenzene-d4	8.088

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, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80



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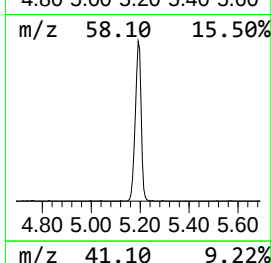
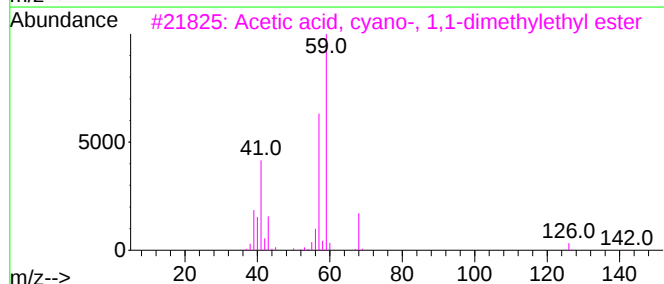
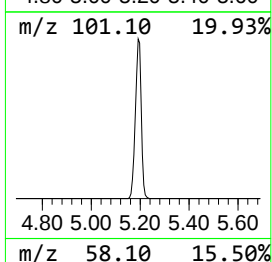
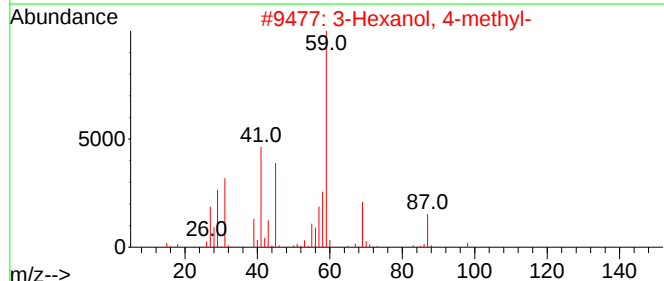
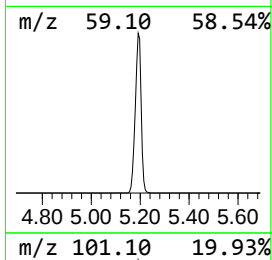
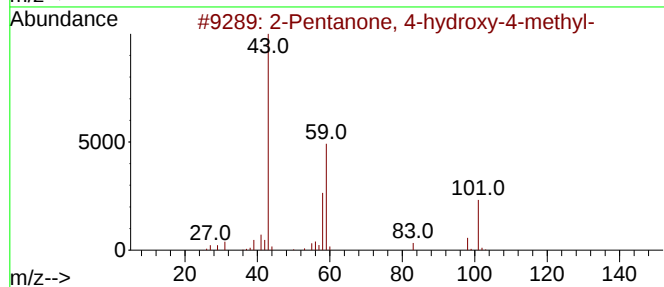
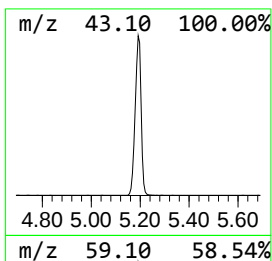
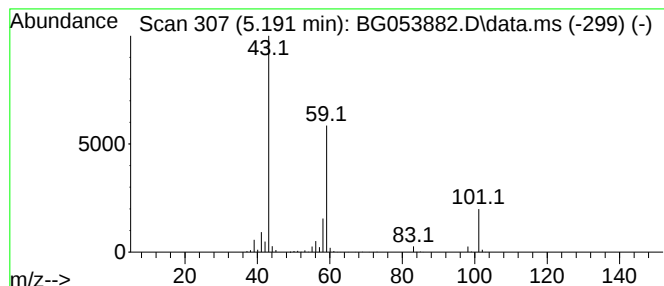
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	254.92 ng	1238130	1,4-Dichlorobenzene-d4	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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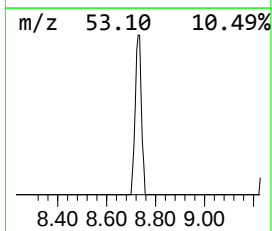
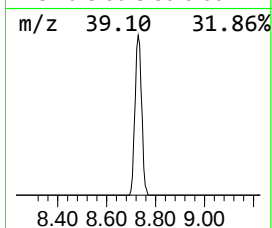
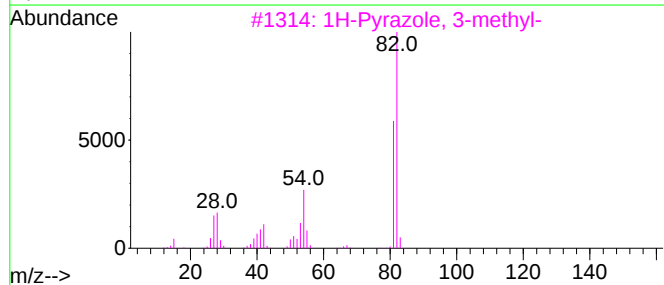
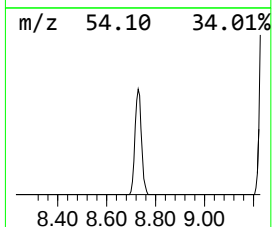
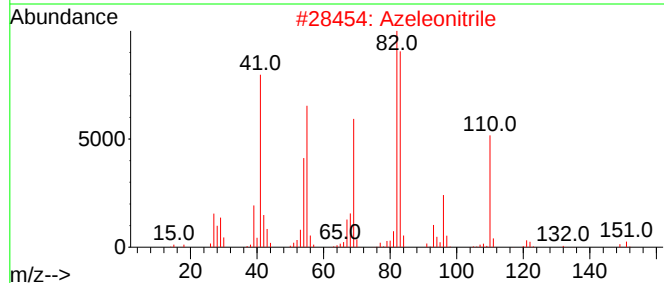
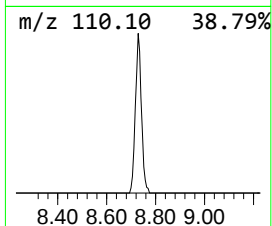
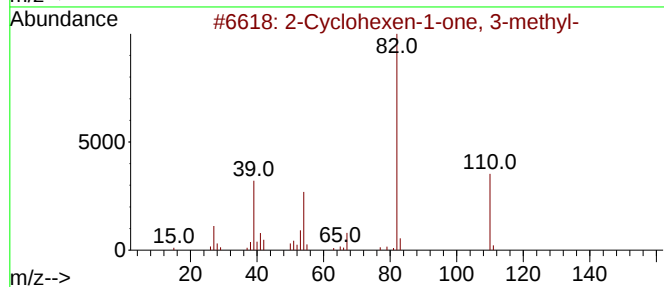
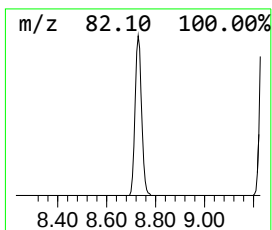
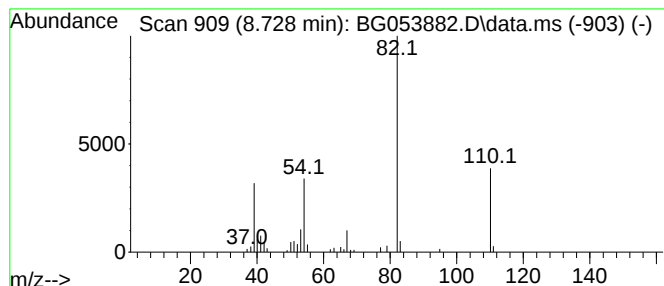
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Peak Number 4 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.728	18.49 ng	89787	1,4-Dichlorobenzene-d4	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2			Azeleoneitrile	150	C9H14N2	001675-69-0	56
3			1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	50
4			2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	40
5			1H-Imidazole, 2-methyl-	82	C4H6N2	000693-98-1	38



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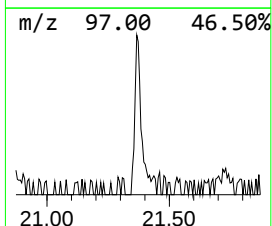
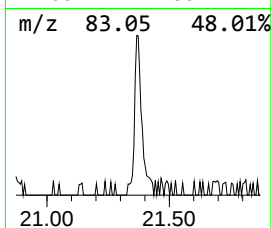
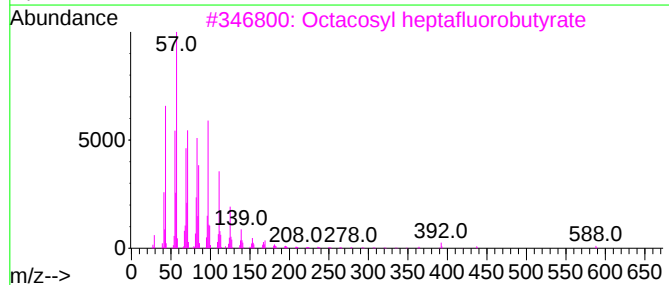
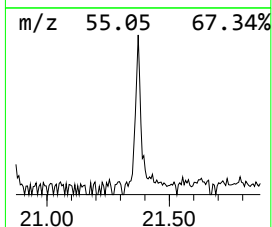
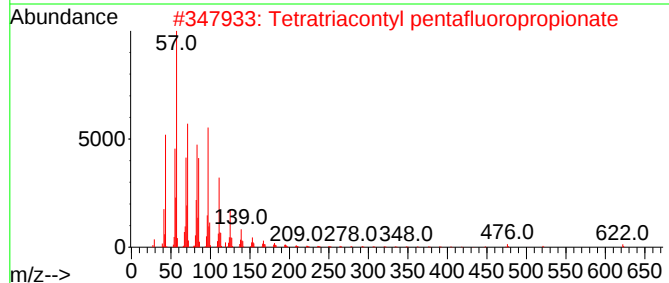
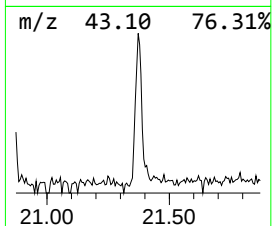
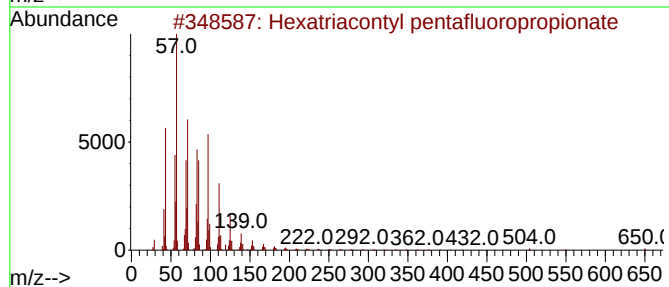
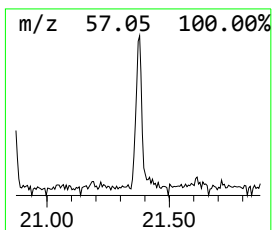
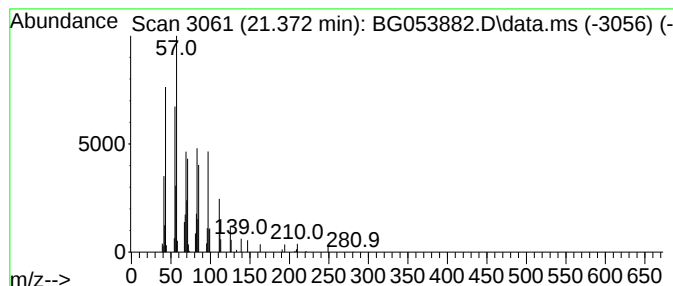
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexatriacontyl pentafluorop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.372	2.72 ng	59315	Chrysene-d12	21.731

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	90
2			Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	90
3			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	87
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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3-Penten-2-one,...	4.598	1024.3	ng	4974660	1	8.088	97138	20.0
2-Pentanone, 4-...	5.191	254.9	ng	1238130	1	8.088	97138	20.0
2-Cyclohexen-1-...	8.728	18.5	ng	89787	1	8.088	97138	20.0
Hexatriacontyl ...	21.372	2.7	ng	59315	5	21.731	435820	20.0