

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG113022\
 Data File : BG055846.D
 Acq On : 30 Nov 2022 17:48
 Operator : CG/JU
 Sample : N5809-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 HOWE-DRUM-B-1129

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055846.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.654	225	232	245	rBV	29410	57773	3.71%	0.580%
2	5.271	330	337	346	rBV	465887	737494	47.31%	7.401%
3	5.753	412	419	437	rBV	610220	1083124	69.48%	10.870%
4	6.370	518	524	533	rVB	35164	58929	3.78%	0.591%
5	7.375	686	695	709	rBV	594925	1128143	72.37%	11.322%
6	8.221	829	839	846	rBV	183146	321764	20.64%	3.229%
7	9.396	1030	1039	1048	rBV	389442	715263	45.88%	7.178%
8	11.047	1310	1320	1329	rBV	236834	440952	28.29%	4.425%
9	13.467	1726	1732	1739	rVB	975240	1504323	96.50%	15.097%
10	14.842	1961	1966	1972	rVB	350298	559994	35.92%	5.620%
11	15.624	2095	2099	2104	rBV4	43540	70715	4.54%	0.710%
12	16.329	2214	2219	2227	rBV	714421	1135352	72.83%	11.394%
13	17.586	2429	2433	2438	rBV	369881	591775	37.96%	5.939%
14	20.183	2872	2875	2880	rVB	1245564	1558837	100.00%	15.644%

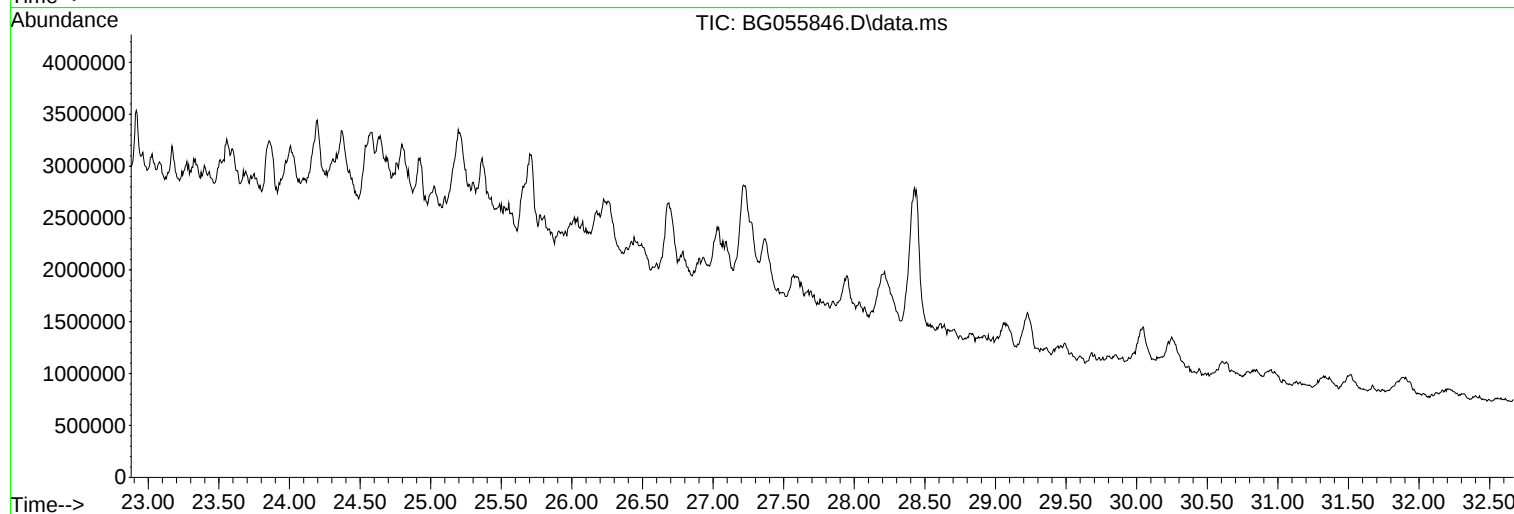
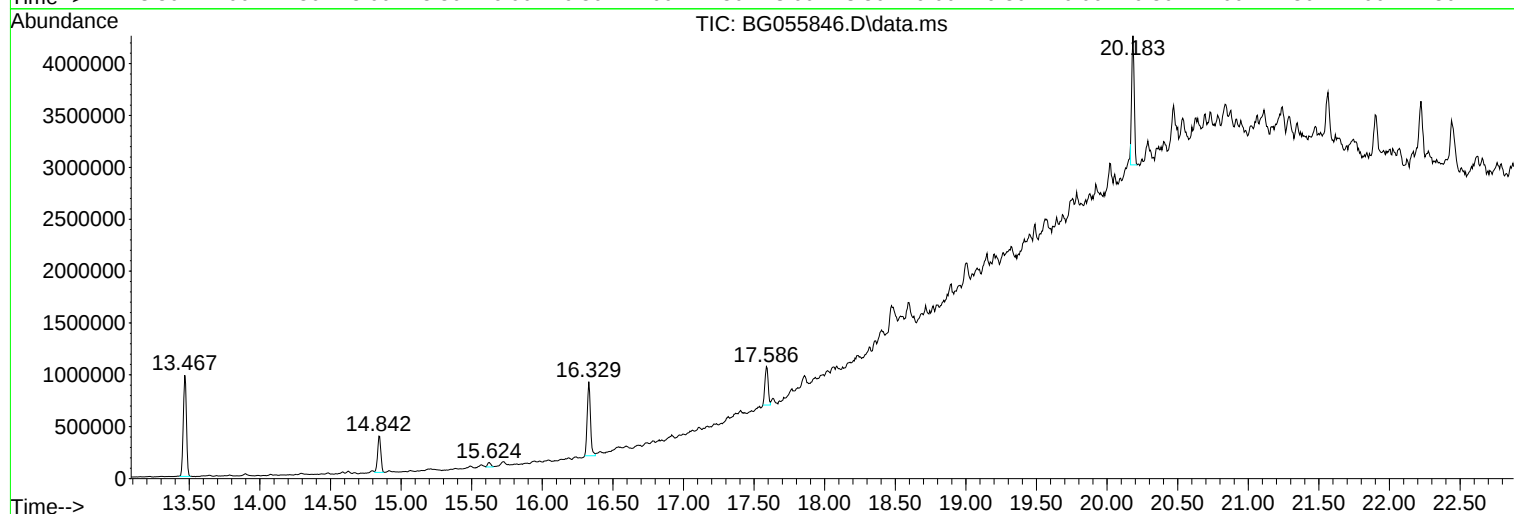
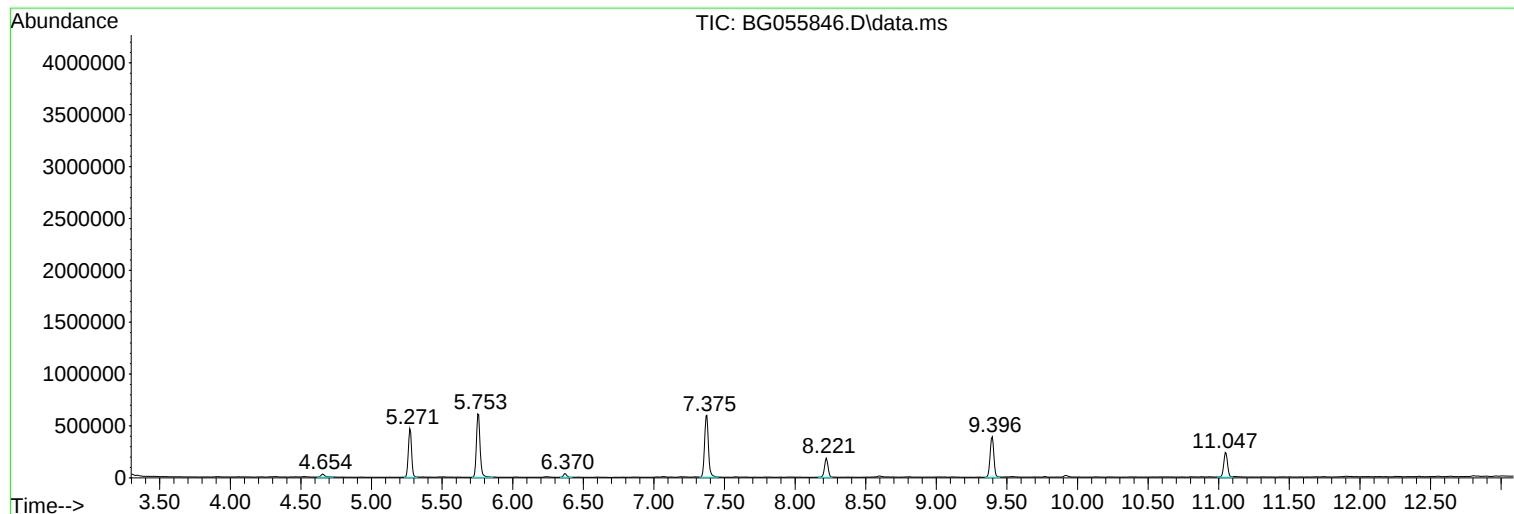
Sum of corrected areas: 9964438

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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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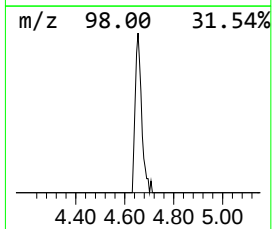
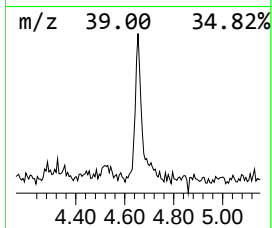
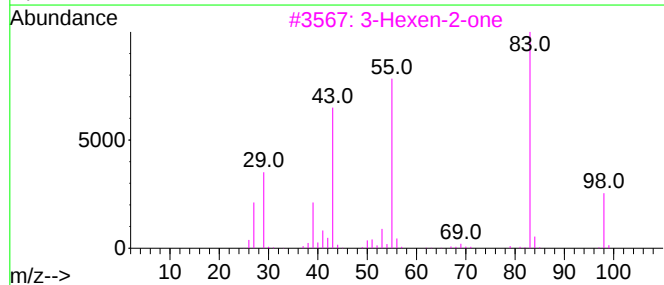
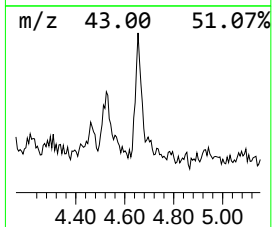
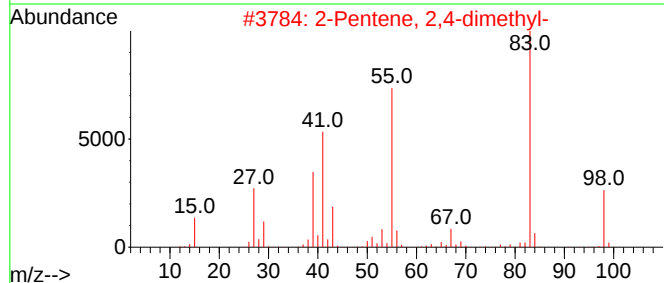
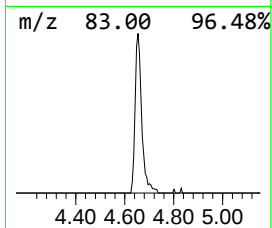
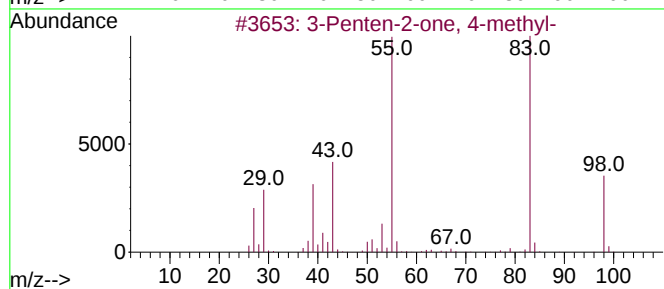
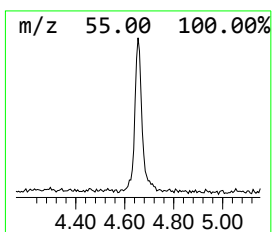
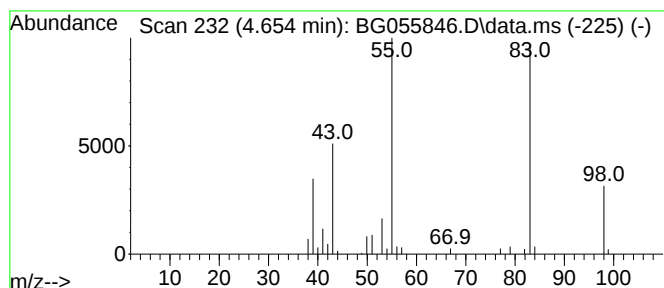
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.654	3.59 ng	57773	1,4-Dichlorobenzene-d4	8.221

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
3		3-Hexen-2-one	98	C6H10O	000763-93-9	78
4		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72



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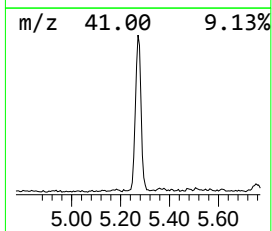
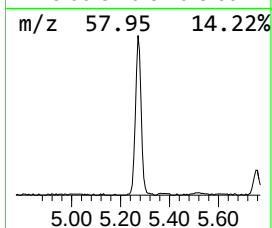
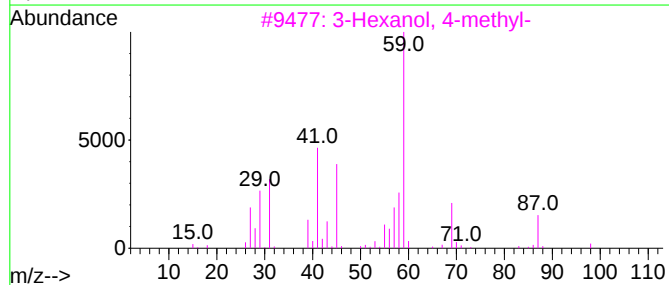
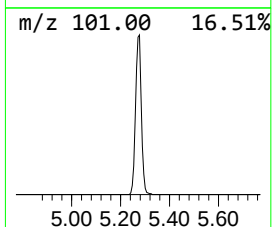
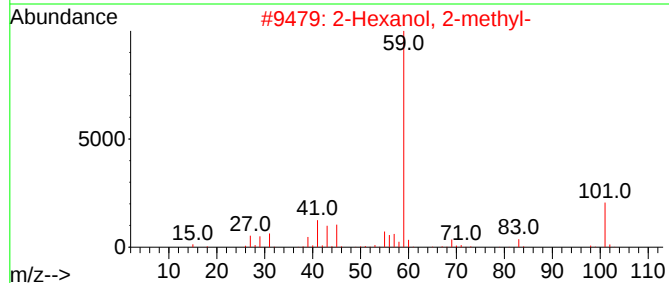
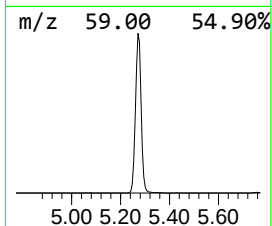
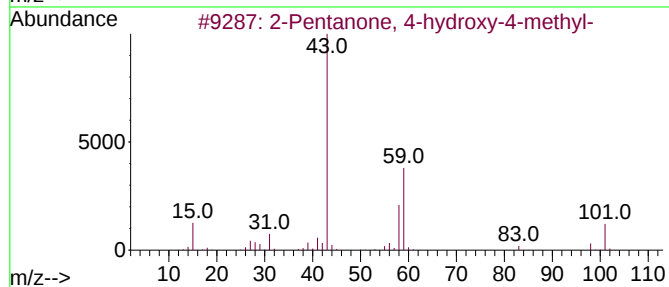
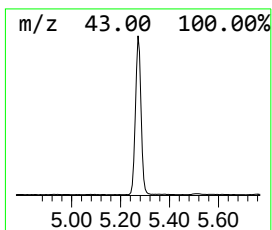
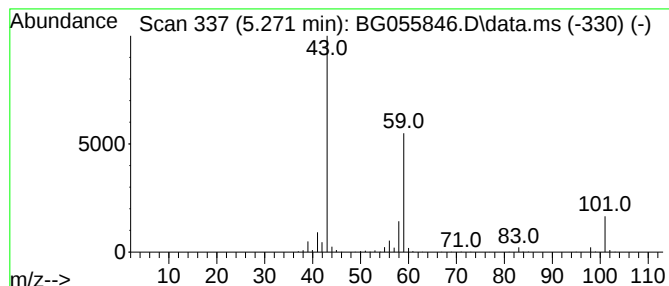
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.271	45.84 ng	737494	1,4-Dichlorobenzene-d4	8.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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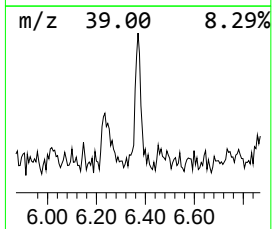
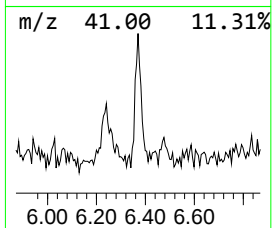
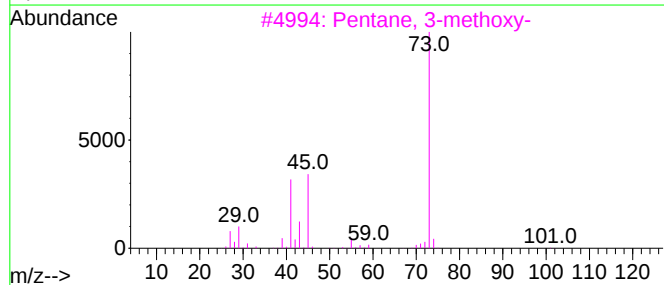
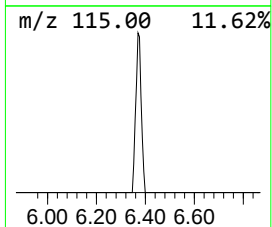
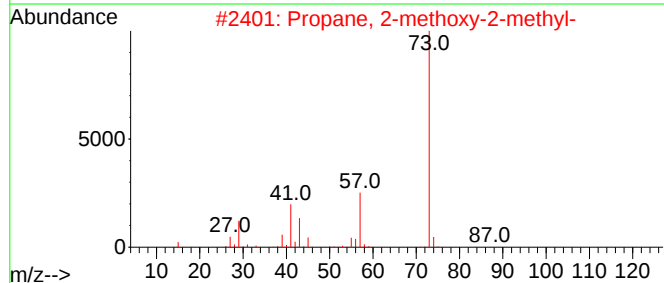
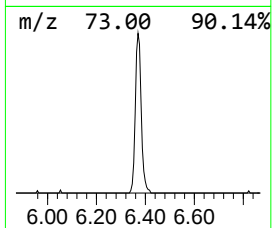
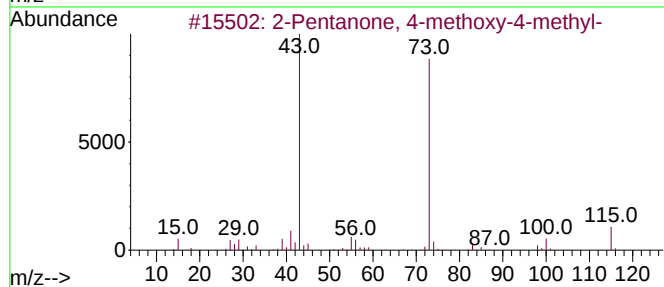
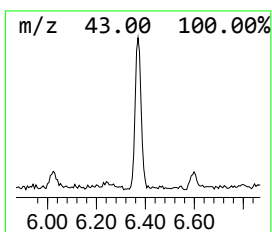
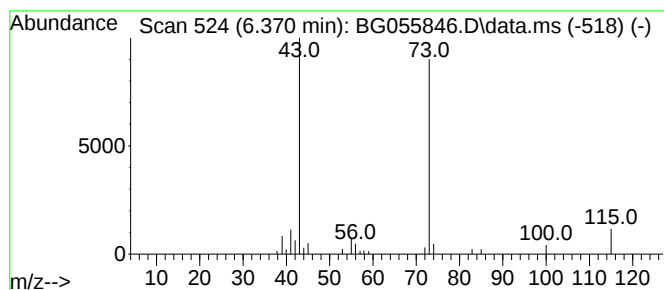
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.370	3.66 ng	58929	1,4-Dichlorobenzene-d4	8.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	14
5			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10



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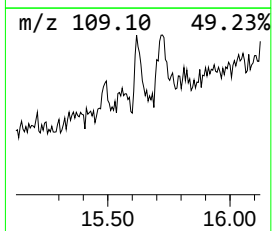
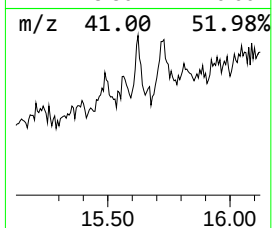
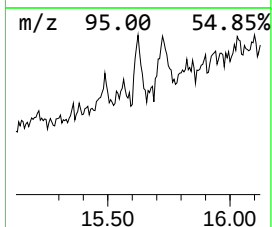
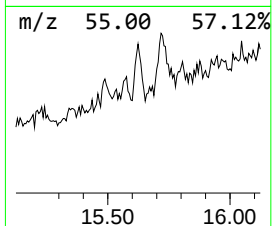
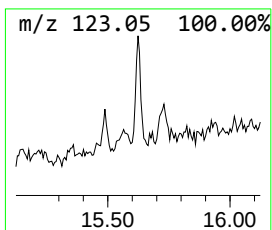
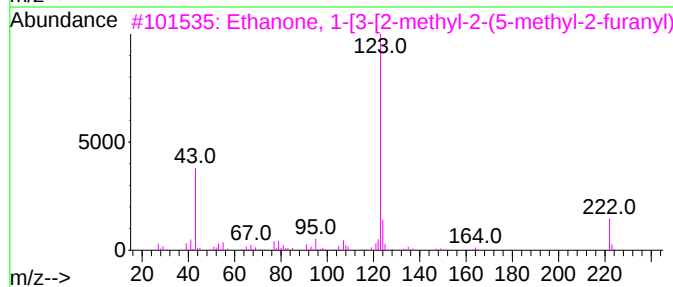
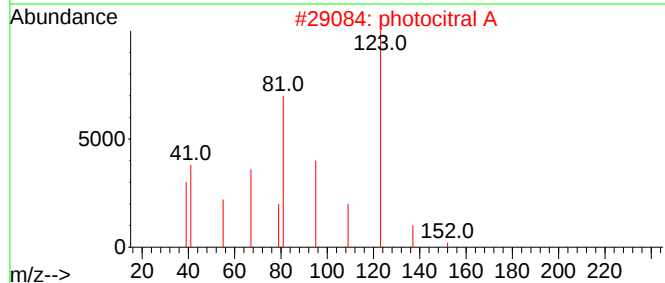
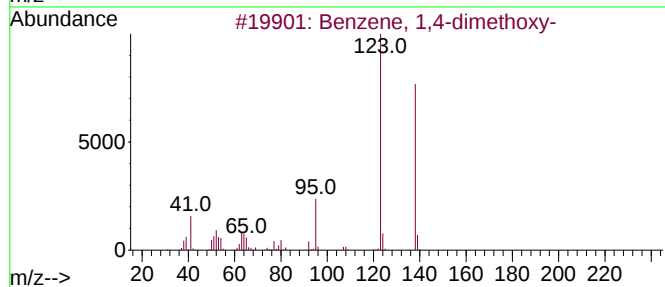
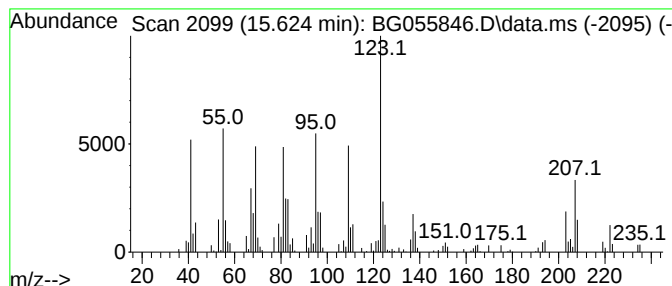
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Peak Number 4 unknown15.624 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.624	2.53 ng	70715	Acenaphthene-d10	14.848

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-dimethoxy-	138	C8H10O2	000150-78-7	43
2			photocitral A	152	C10H16O	055253-28-6	38
3			Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	38
4			Salvial-4(14)-en-1-one	220	C15H24O	073809-82-2	27
5			(Phenylthio)acetic acid, cyclobu...	222	C12H14O2S	1010299-95-5	27



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.654	3.6	ng	57773	1	8.221	321764	20.0
2-Pentanone, 4-...	5.271	45.8	ng	737494	1	8.221	321764	20.0
2-Pentanone, 4-...	6.370	3.7	ng	58929	1	8.221	321764	20.0
unknown15.624	15.624	2.5	ng	70715	3	14.848	559994	20.0