

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
 Data File : BG055607.D
 Acq On : 14 Nov 2022 16:42
 Operator : CG/JU
 Sample : N5554-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RBR251374

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055607.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.704	235	241	247	rBV	31510	51322	1.44%	0.288%
2	5.321	339	346	355	rBV	325104	514019	14.40%	2.886%
3	5.797	419	427	440	rBV	1067419	1731337	48.52%	9.720%
4	7.407	692	701	717	rVB	1080473	1902592	53.32%	10.682%
5	8.265	838	847	854	rBV	200614	343271	9.62%	1.927%
6	9.434	1038	1046	1055	rBV	642174	1170015	32.79%	6.569%
7	9.769	1097	1103	1109	rBV2	36980	59379	1.66%	0.333%
8	10.838	1277	1285	1297	rBV	62730	125907	3.53%	0.707%
9	11.097	1319	1329	1336	rBV	289709	518463	14.53%	2.911%
10	13.512	1733	1740	1747	rBV	1794512	2814816	78.88%	15.803%
11	14.041	1826	1830	1833	rBV5	39633	64485	1.81%	0.362%
12	14.082	1834	1837	1842	rVB3	53956	71936	2.02%	0.404%
13	14.170	1846	1852	1857	rBV2	207649	358823	10.06%	2.015%
14	14.887	1969	1974	1981	rVB	474064	788330	22.09%	4.426%
15	16.373	2222	2227	2237	rBV	1261841	2065485	57.88%	11.596%
16	20.227	2878	2883	2890	rVB	2468497	3568461	100.00%	20.034%
17	21.937	3170	3174	3180	rVB	482007	840250	23.55%	4.717%
18	25.363	3750	3757	3768	rVB	277098	822694	23.05%	4.619%

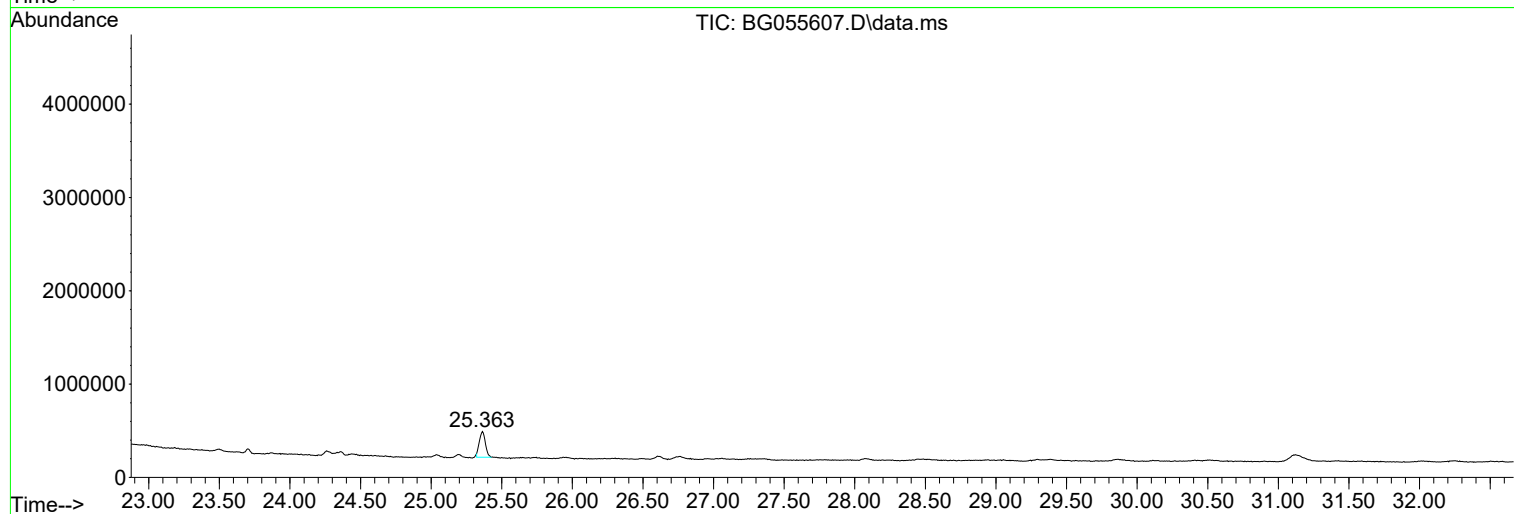
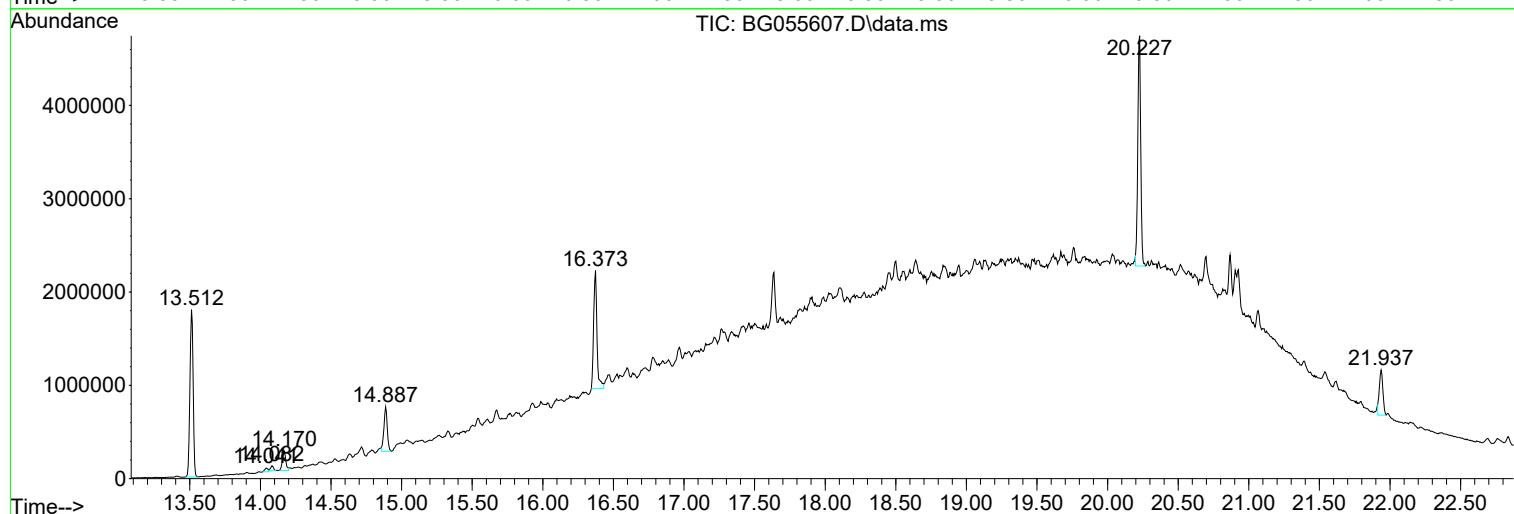
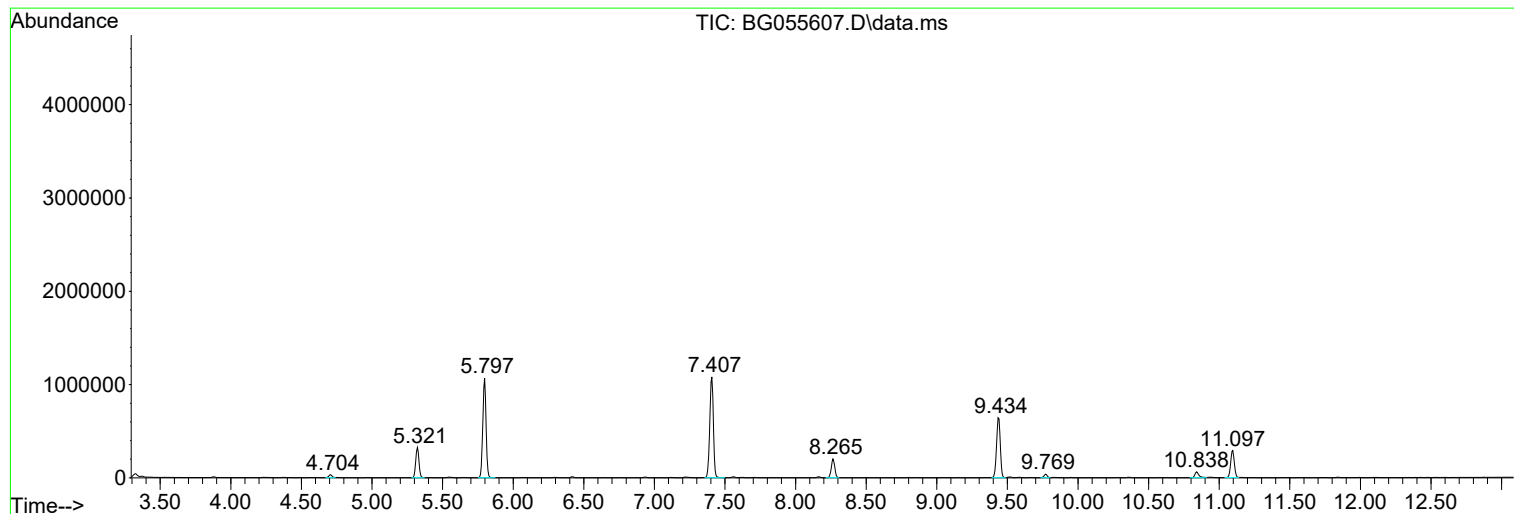
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG055607.D
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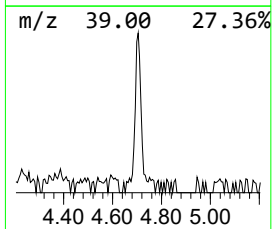
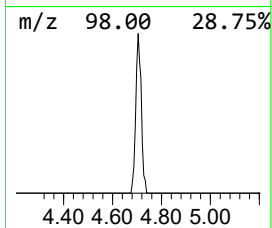
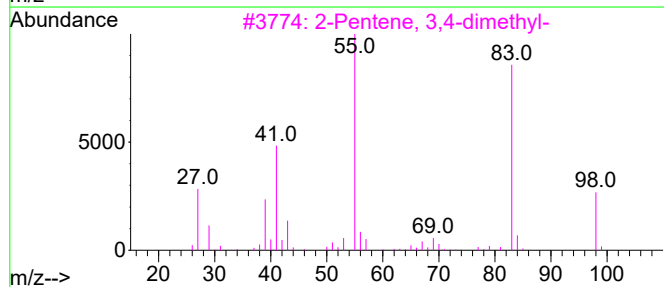
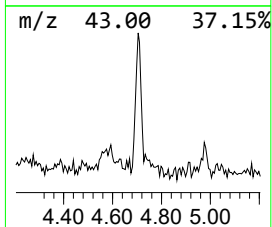
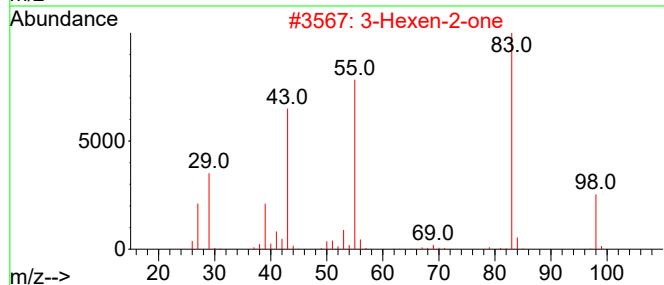
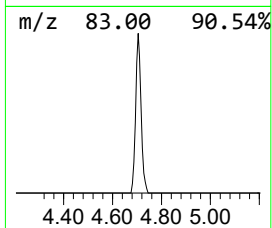
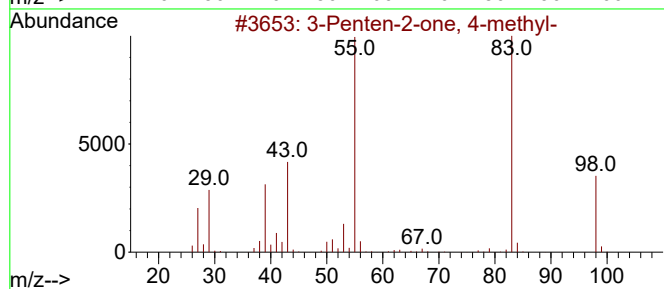
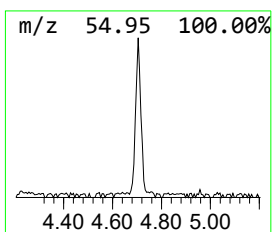
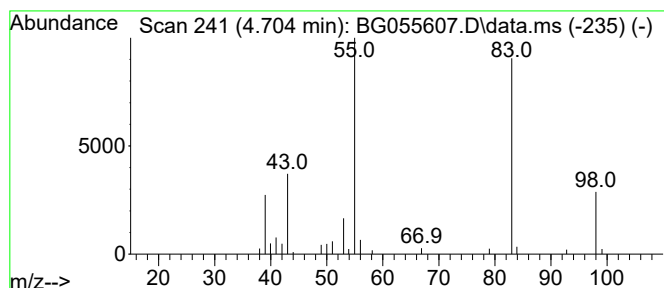
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.704	2.99 ng	51322	1,4-Dichlorobenzene-d4	8.265

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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-	98	C7H14	024910-63-2	80
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5			2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	72



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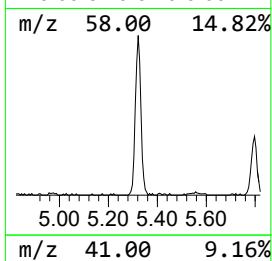
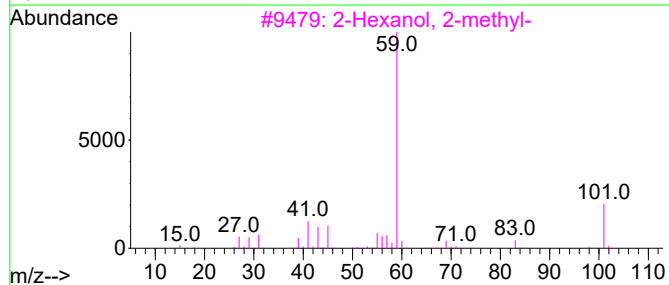
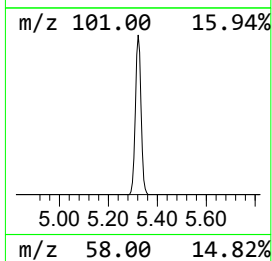
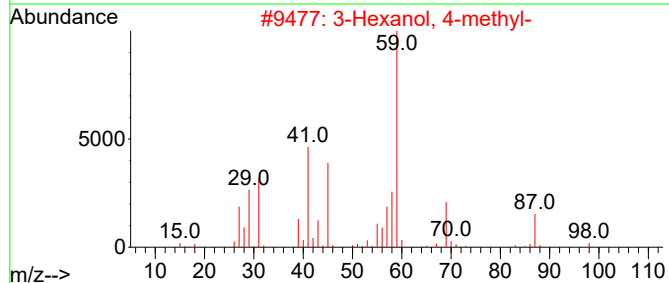
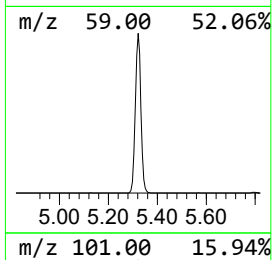
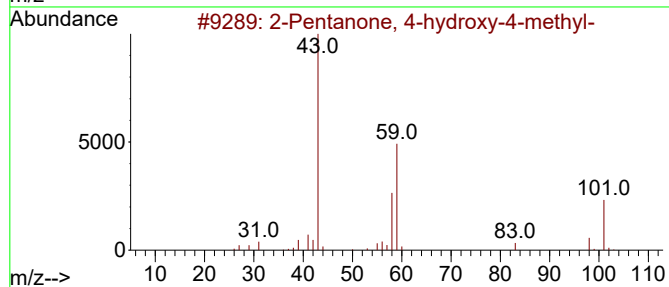
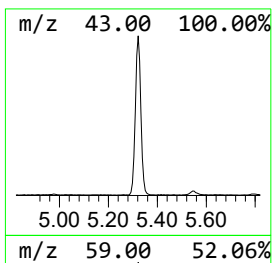
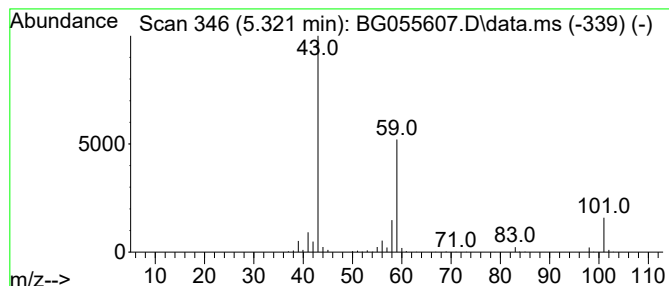
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.321	29.95 ng	514019	1,4-Dichlorobenzene-d4			8.265
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	33
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	28
4	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	25
5	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25



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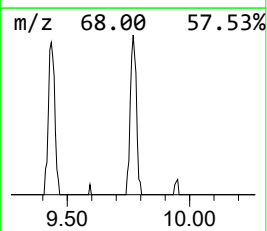
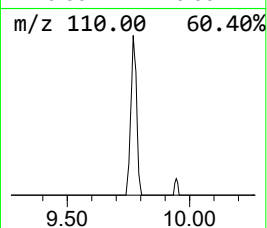
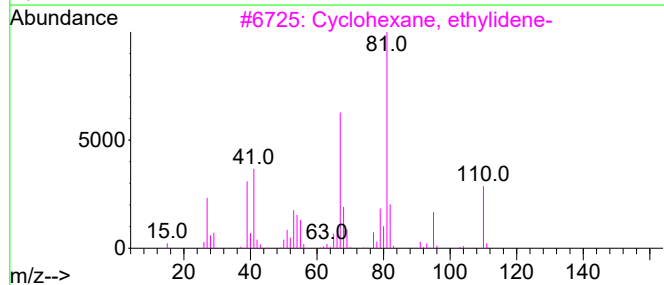
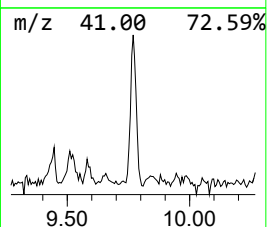
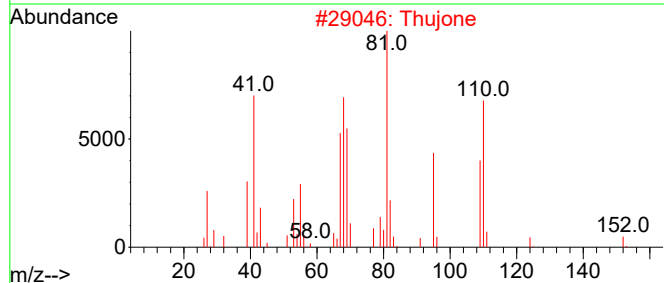
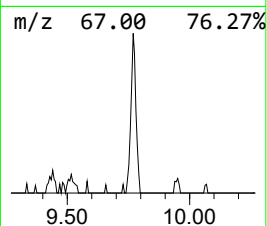
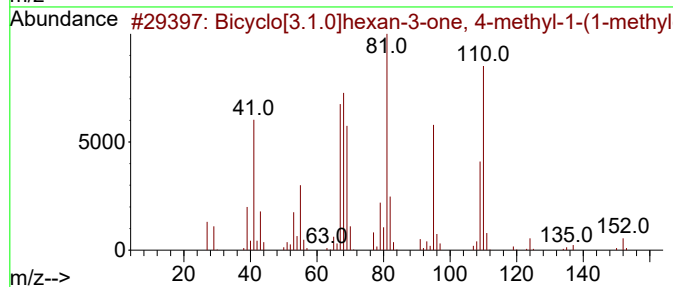
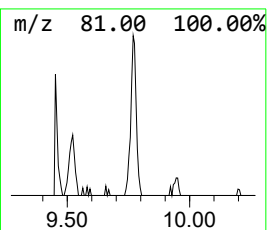
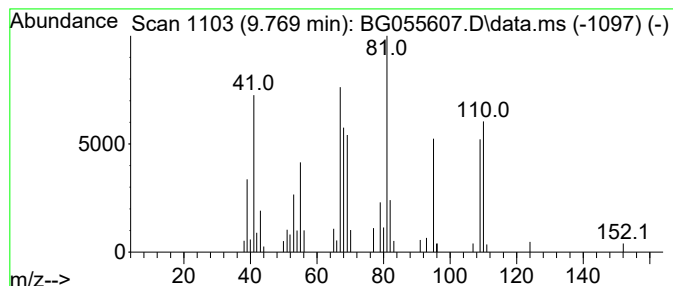
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Bicyclo[3.1.0]hexan-3-one, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.769	2.29 ng	59379	Naphthalene-d8	11.097

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	001125-12-8	90
2		Thujone	152	C10H16O	000546-80-5	81
3		Cyclohexane, ethylidene-	110	C8H14	001003-64-1	52
4		Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	49
5		1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	46



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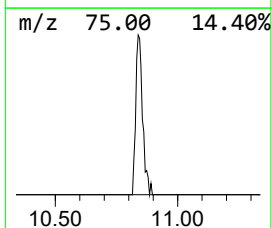
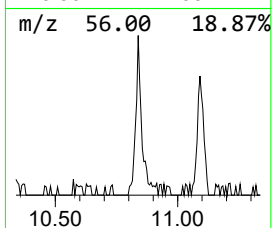
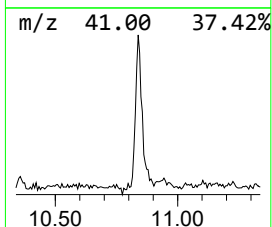
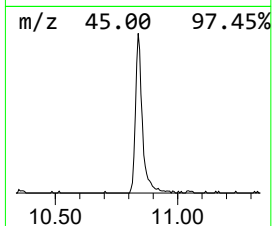
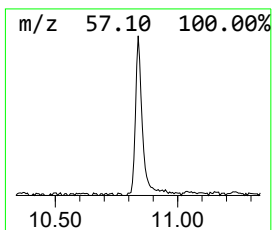
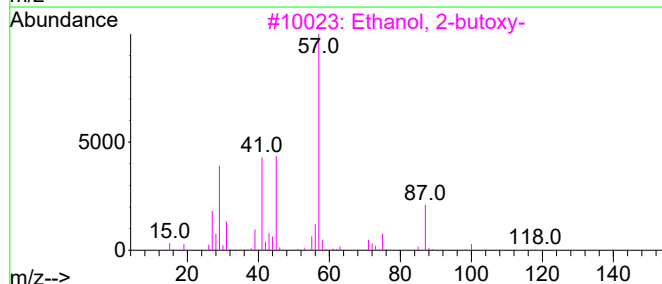
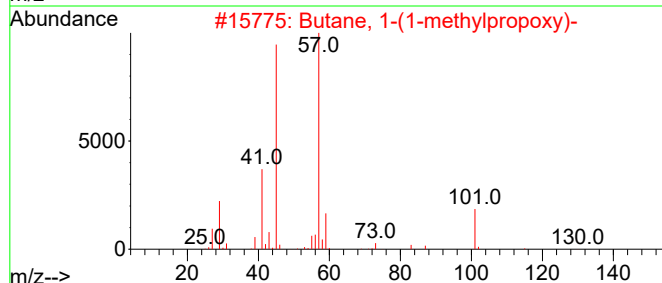
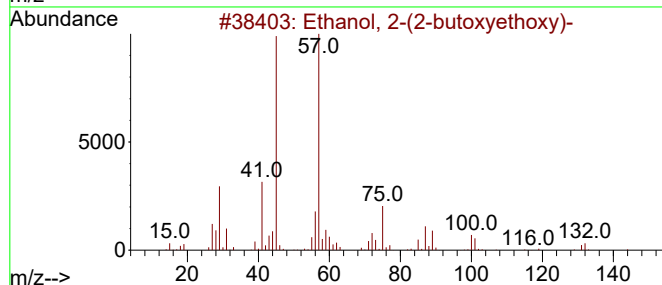
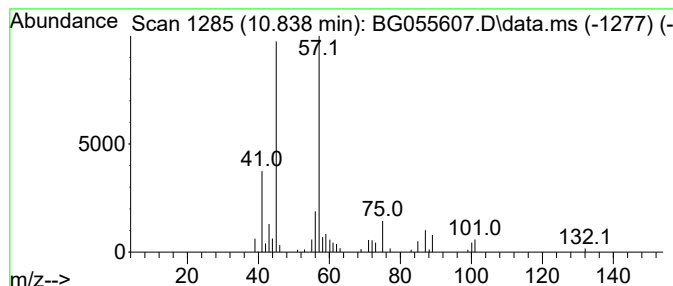
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.838	4.86 ng	125907	Naphthalene-d8	11.097

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
3			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	53
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	53



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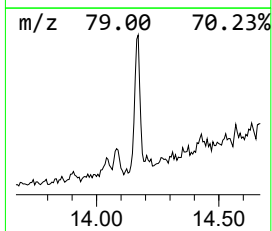
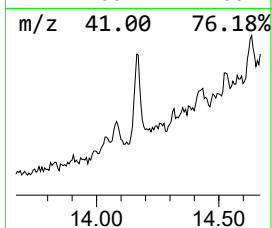
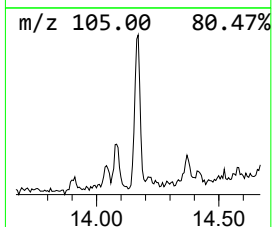
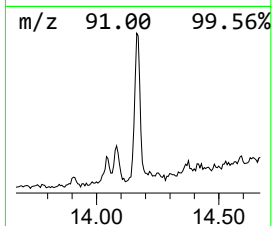
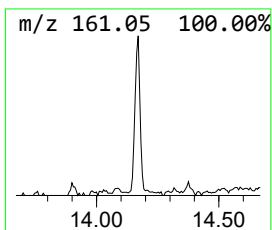
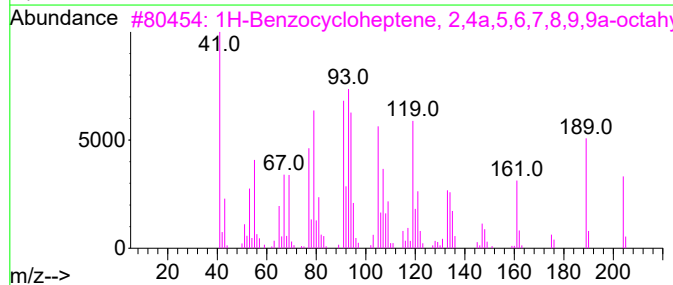
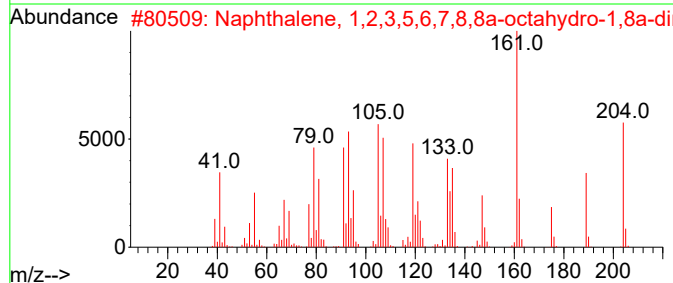
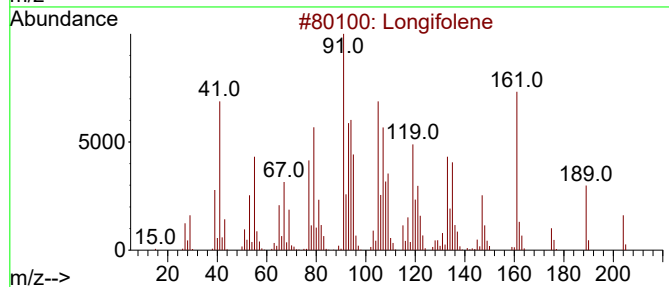
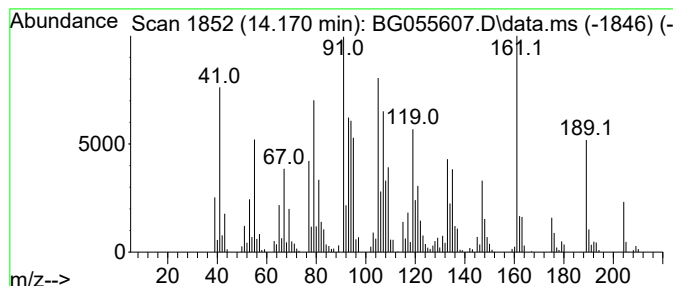
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Longifolene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.170	9.10 ng	358823	Acenaphthene-d10	14.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Longifolene	204	C15H24	000475-20-7	99
2			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	95
3			1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	003853-83-6	86
4			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	83
5			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	83



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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,...	4.704	3.0	ng	51322	1	8.265	343271	20.0
2-Pentanone, 4-...	5.321	29.9	ng	514019	1	8.265	343271	20.0
Bicyclo[3.1.0]h...	9.769	2.3	ng	59379	2	11.097	518463	20.0
Ethanol, 2-(2-b...	10.838	4.9	ng	125907	2	11.097	518463	20.0
Longifolene	14.170	9.1	ng	358823	3	14.887	788330	20.0