

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
 Data File : BF131449.D
 Acq On : 29 Nov 2022 01:49
 Operator : CG\JU
 Sample : N5752-03 5X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-8S

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_F\Methods\8270-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131449.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	15	20	25	rVB	130773	166929	19.12%	2.942%
2	2.593	77	86	92	rVB	84055	127566	14.61%	2.248%
3	5.157	519	522	526	rBV	64627	65926	7.55%	1.162%
4	5.557	583	590	594	rBV	438623	389738	44.63%	6.868%
5	6.569	758	762	765	rBV	345104	271559	31.10%	4.785%
6	6.957	824	828	831	rBV	566582	437956	50.15%	7.717%
7	7.516	915	923	926	rBV	169571	144110	16.50%	2.539%
8	8.245	1043	1047	1050	rBV	966049	741470	84.91%	13.066%
9	9.322	1227	1230	1233	rBV	731030	530525	60.76%	9.349%
10	9.469	1250	1255	1259	rBV7	19053	36214	4.15%	0.638%
11	9.822	1312	1315	1317	rVB3	44702	36845	4.22%	0.649%
12	9.875	1320	1324	1325	rBV2	89880	84594	9.69%	1.491%
13	9.892	1325	1327	1330	rVB2	84292	63288	7.25%	1.115%
14	10.010	1344	1347	1350	rVB	1105334	873218	100.00%	15.388%
15	10.045	1350	1353	1354	rBV	80241	83257	9.53%	1.467%
16	10.122	1364	1366	1368	rBV3	47412	42207	4.83%	0.744%
17	10.386	1409	1411	1414	rVB3	59443	48075	5.51%	0.847%
18	10.416	1414	1416	1420	rBV5	82033	90771	10.39%	1.600%
19	10.469	1422	1425	1430	rVV	184867	217049	24.86%	3.825%
20	10.798	1479	1481	1486	rBV	328879	380041	43.52%	6.697%
21	11.510	1599	1602	1605	rBV	939973	843505	96.60%	14.864%

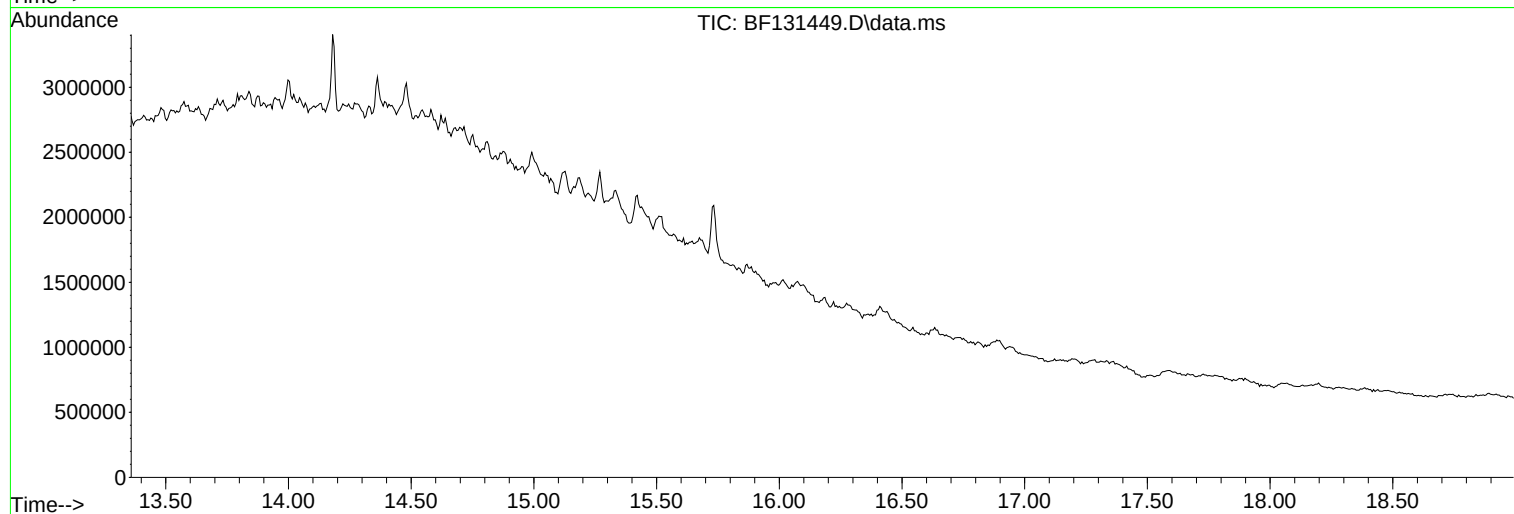
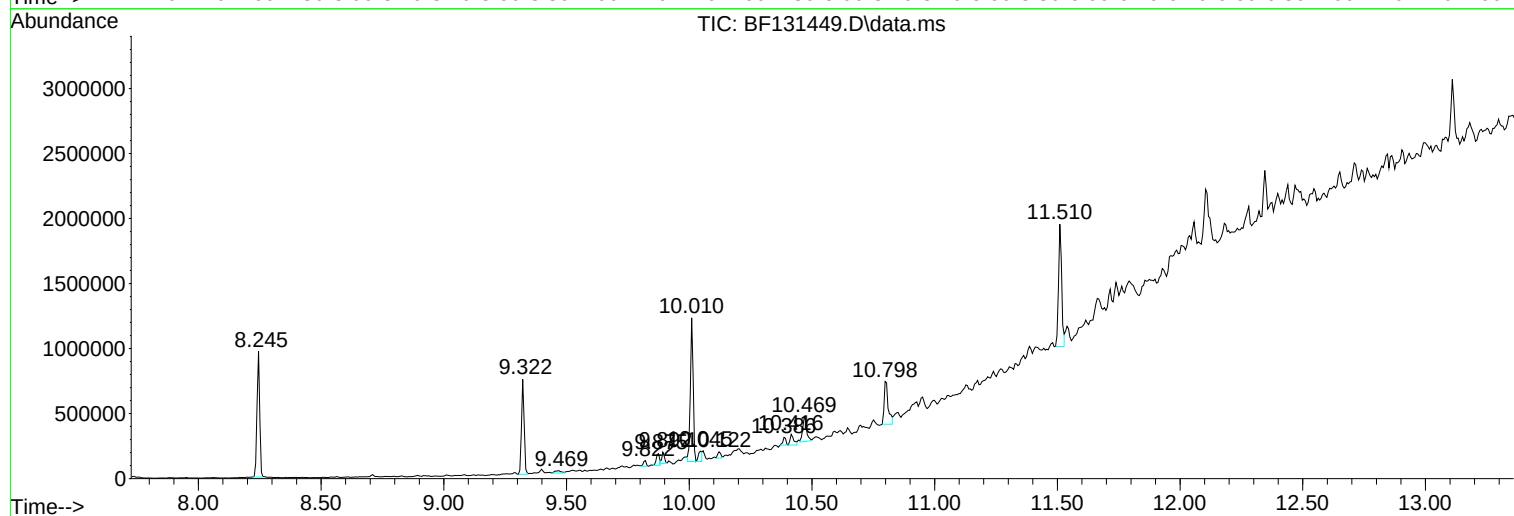
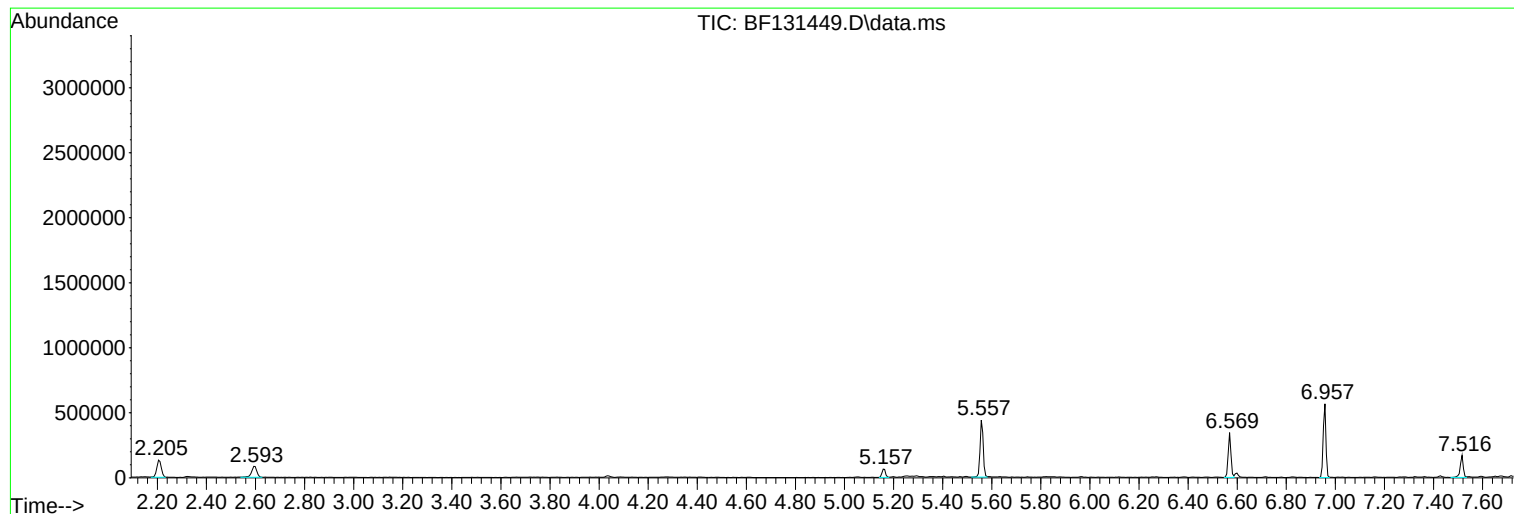
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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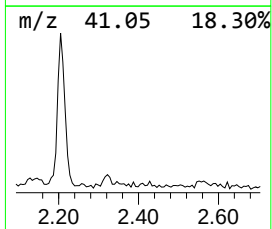
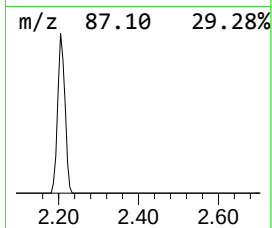
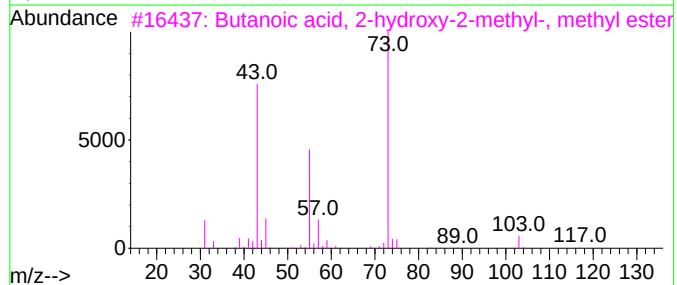
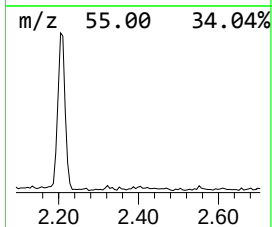
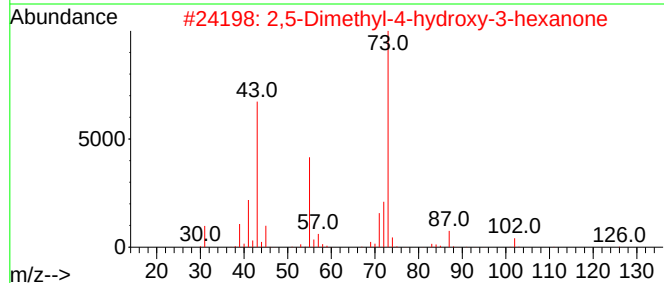
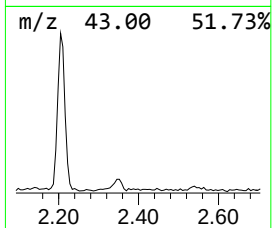
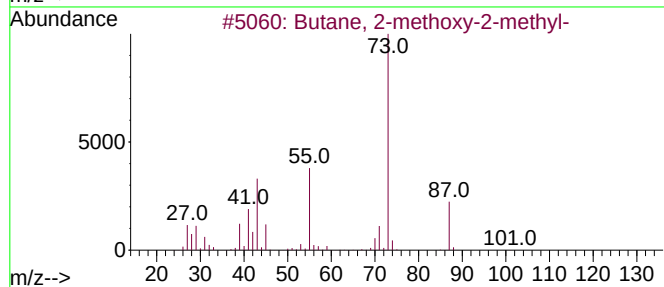
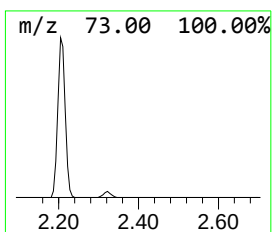
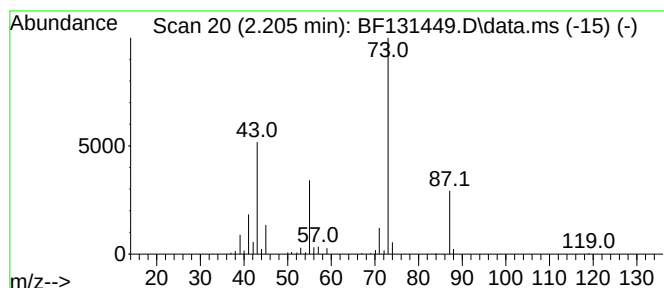
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	7.62 ng	166929	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	50
3			Butanoic acid, 2-hydroxy-2-methyl...	132	C6H12O3	032793-34-3	43
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	42
5			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40



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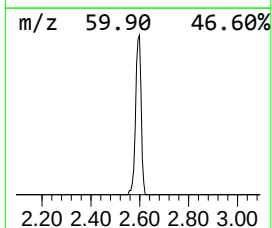
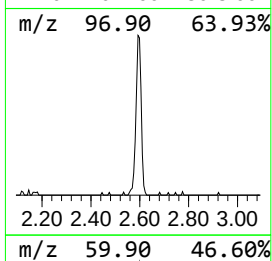
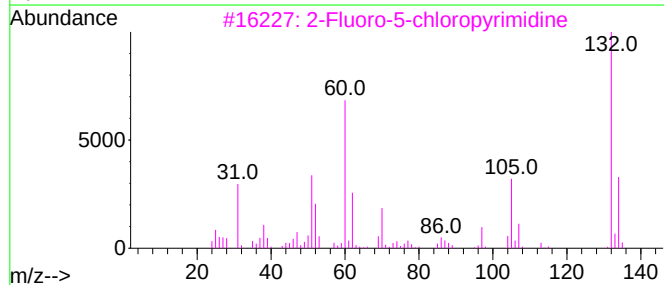
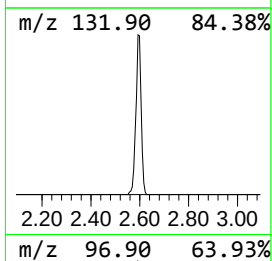
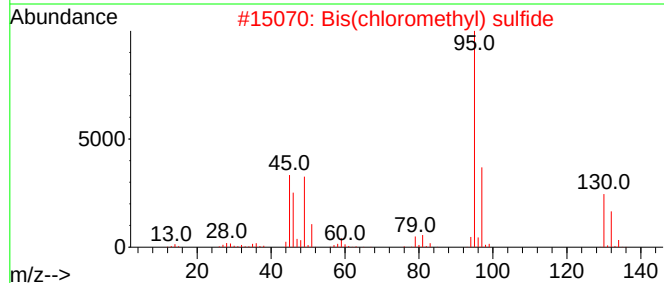
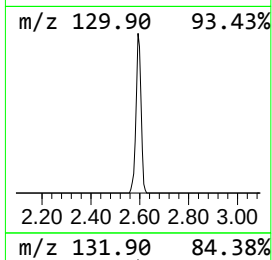
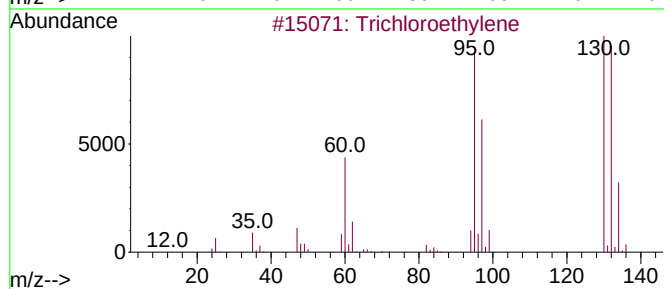
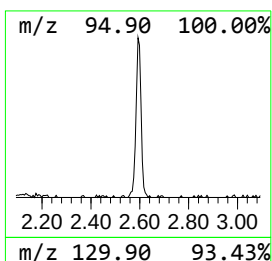
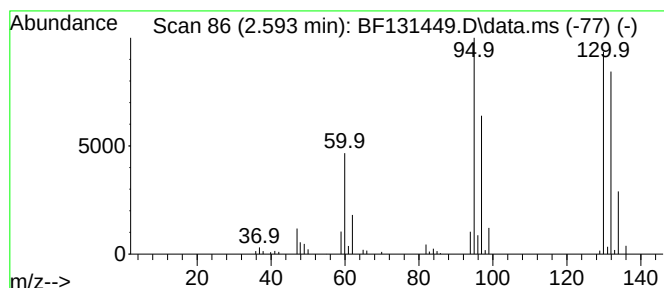
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Trichloroethylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.593	5.83 ng	127566	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroethylene	130	C2HCl3	000079-01-6	98
2			Bis(chloromethyl) sulfide	130	C2H4Cl2S	003592-44-7	58
3			2-Fluoro-5-chloropyrimidine	132	C4H2ClFN2	062802-37-3	35
4			1H-1,2,4-Triazol-3-amine, 5-(met...	130	C3H6N4S	045534-08-5	12
5			1,3-Oxathiane, 4,6-dimethyl-, tr...	132	C6H12OS	022452-26-2	10



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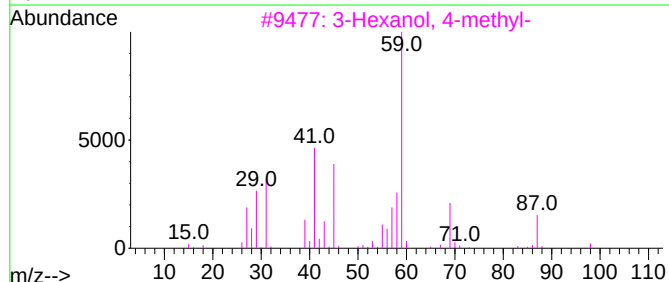
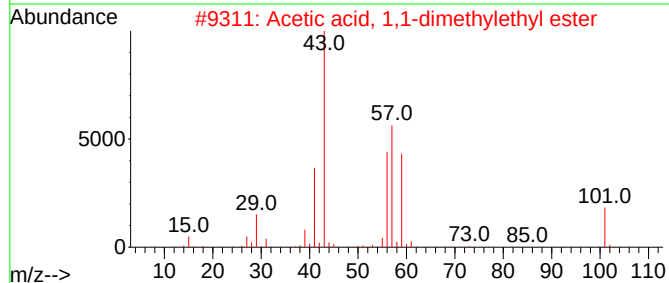
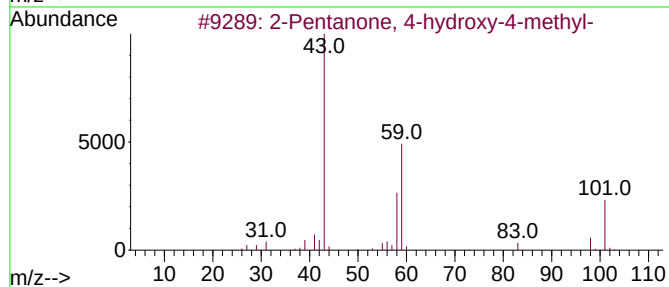
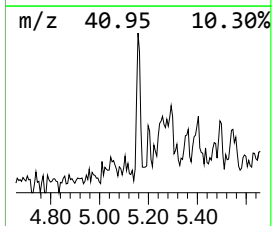
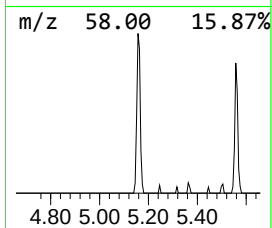
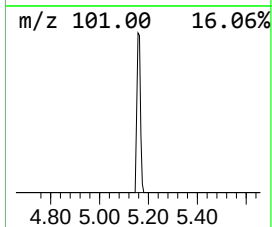
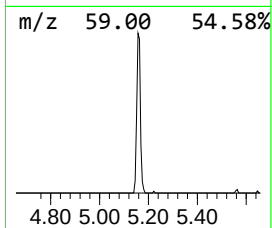
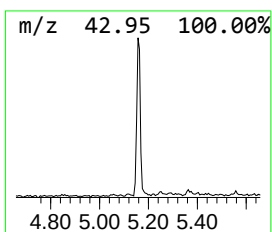
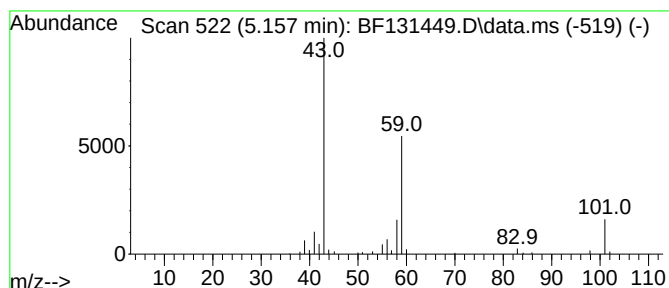
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	3.01 ng	65926	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	38
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
5			3-Octanol	130	C8H18O	000589-98-0	28



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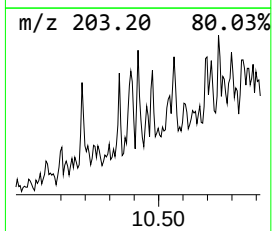
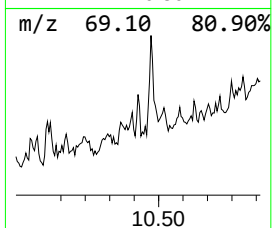
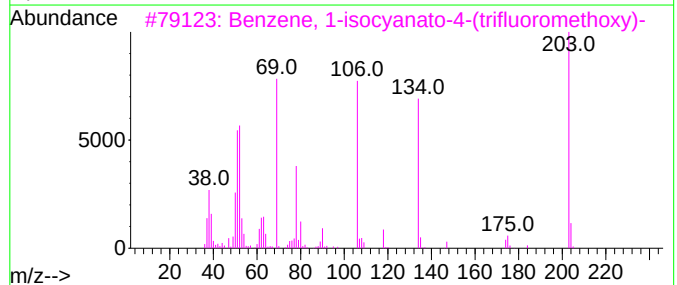
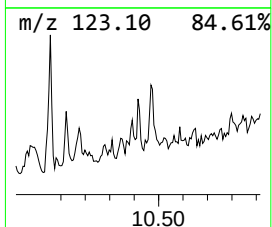
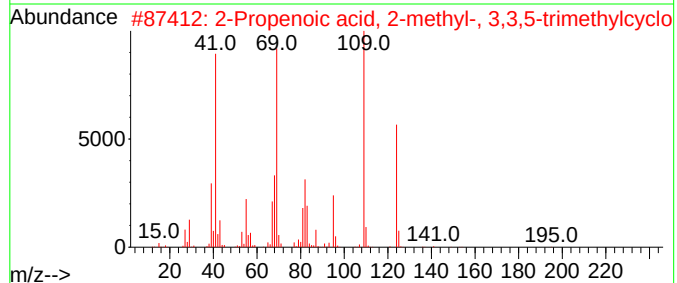
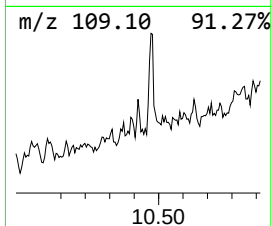
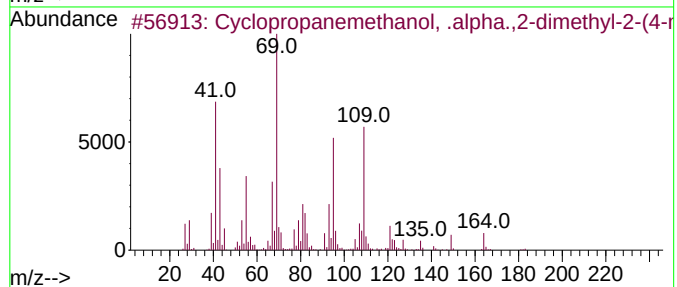
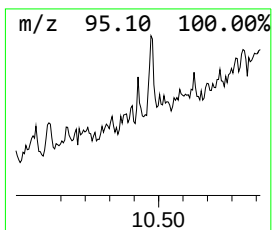
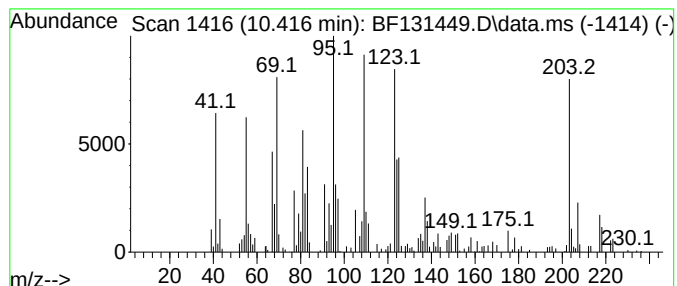
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown10.416 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.416	2.08 ng	90771	Acenaphthene-d10	10.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	35
2			2-Propenoic acid, 2-methyl-, 3,3...	210	C13H22O2	007779-31-9	27
3			Benzene, 1-isocyanato-4-(trifluo...	203	C8H4F3NO2	035037-73-1	18
4			Bicyclo[3.3.1]nonan-9-one, 2,4-d...	211	C11H17NO3	129967-64-2	14
5			3,7-Dimethyloct-6-ene-1,2,3-triol	188	C10H20O3	065180-52-1	14



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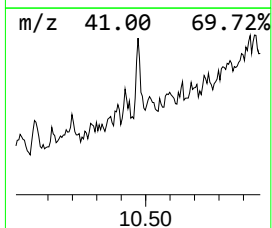
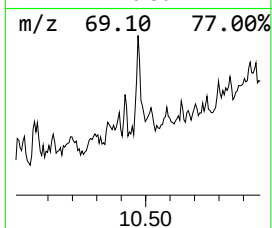
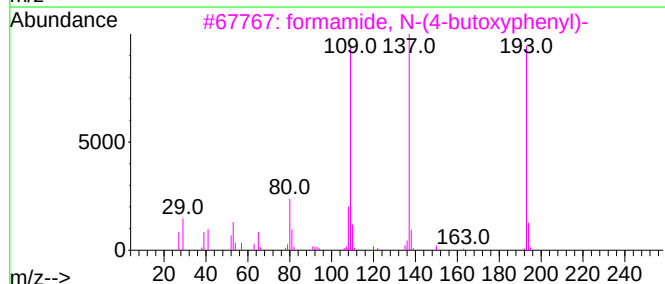
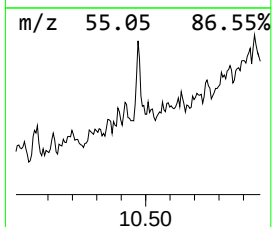
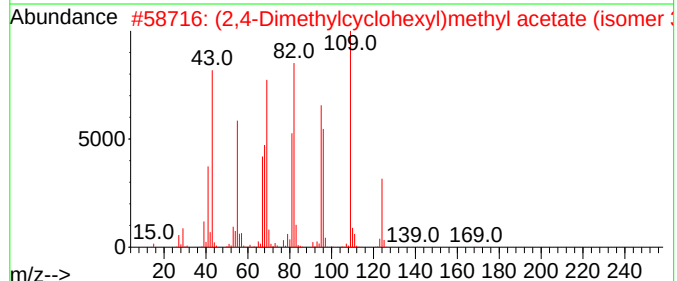
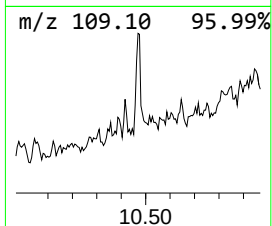
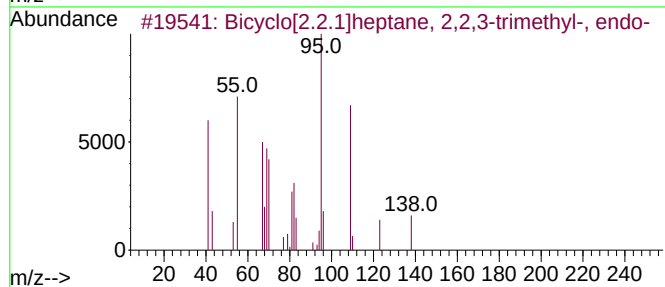
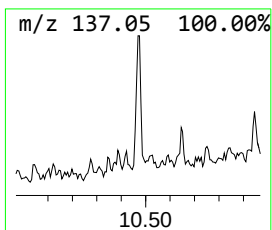
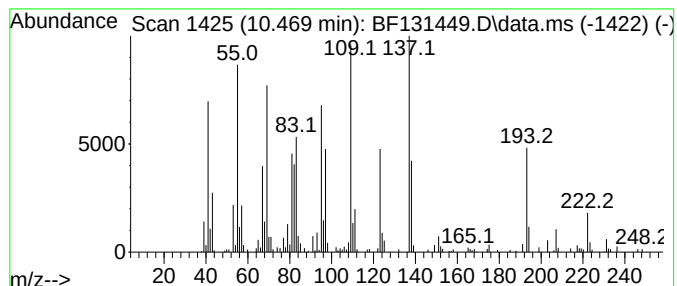
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown10.469 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	4.97 ng	217049	Acenaphthene-d10	10.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	38
2			(2,4-Dimethylcyclohexyl)methyl a...	184	C11H20O2	1000497-97-0	35
3			formamide, N-(4-butoxyphenyl)-	193	C11H15NO2	1000400-28-0	35
4			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	30
5			6-Octen-1-ol, 3,7-dimethyl-, ace...	198	C12H22O2	000150-84-5	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.205	7.6	ng	166929	1	6.957	437956	20.0
Trichloroethylene	2.593	5.8	ng	127566	1	6.957	437956	20.0
2-Pentanone, 4-...	5.157	3.0	ng	65926	1	6.957	437956	20.0
unknown10.416	10.416	2.1	ng	90771	3	10.010	873218	20.0
unknown10.469	10.469	5.0	ng	217049	3	10.010	873218	20.0