

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091924\
 Data File : BF139466.D
 Acq On : 19 Sep 2024 16:03
 Operator : RC/JU
 Sample : P4088-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-614-COMP-08

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-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139466.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	9	16	24	rVB	719331	1117285	68.80%	9.180%
2	5.093	501	510	521	rBV	123106	182644	11.25%	1.501%
3	5.498	573	579	584	rBV	1029400	1364541	84.02%	11.212%
4	6.504	743	750	755	rBV	1116507	1501190	92.43%	12.335%
5	6.875	808	813	818	rVB	372178	458865	28.25%	3.770%
6	7.440	902	909	914	rBV	721894	946968	58.31%	7.781%
7	7.692	947	952	957	rVB	19361	24565	1.51%	0.202%
8	8.157	1026	1031	1036	rBV	462196	570519	35.13%	4.688%
9	8.375	1064	1068	1074	rVB2	14844	17635	1.09%	0.145%
10	9.234	1208	1214	1219	rBV	1296151	1624056	100.00%	13.344%
11	9.910	1324	1329	1334	rBV	500153	604160	37.20%	4.964%
12	10.622	1445	1450	1458	rBV	283736	346285	21.32%	2.845%
13	10.698	1458	1463	1474	rVV	705302	883405	54.39%	7.259%
14	10.933	1498	1503	1511	rVB	50390	66453	4.09%	0.546%
15	11.392	1576	1581	1588	rBV	458495	582354	35.86%	4.785%
16	11.916	1665	1670	1675	rBV2	20303	29312	1.80%	0.241%
17	12.980	1845	1851	1856	rBV	886101	1150826	70.86%	9.456%
18	13.886	1999	2005	2018	rBV3	19810	61961	3.82%	0.509%
19	14.027	2024	2029	2038	rVB	242473	315463	19.42%	2.592%
20	15.498	2273	2279	2294	rBV	202472	321998	19.83%	2.646%

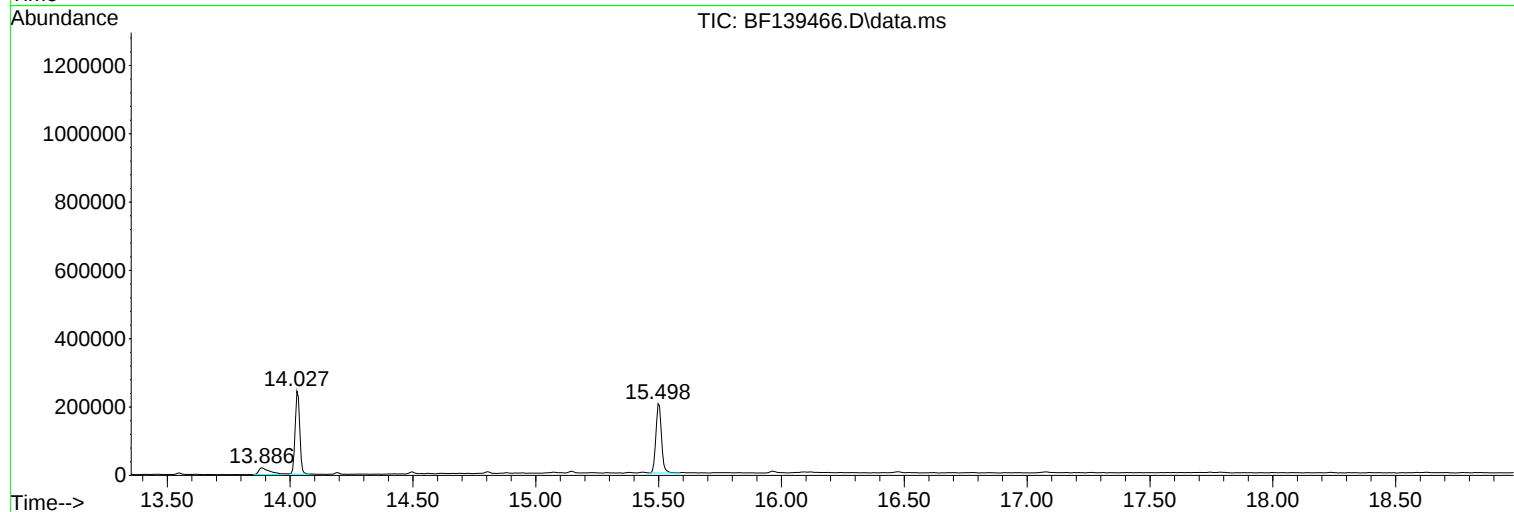
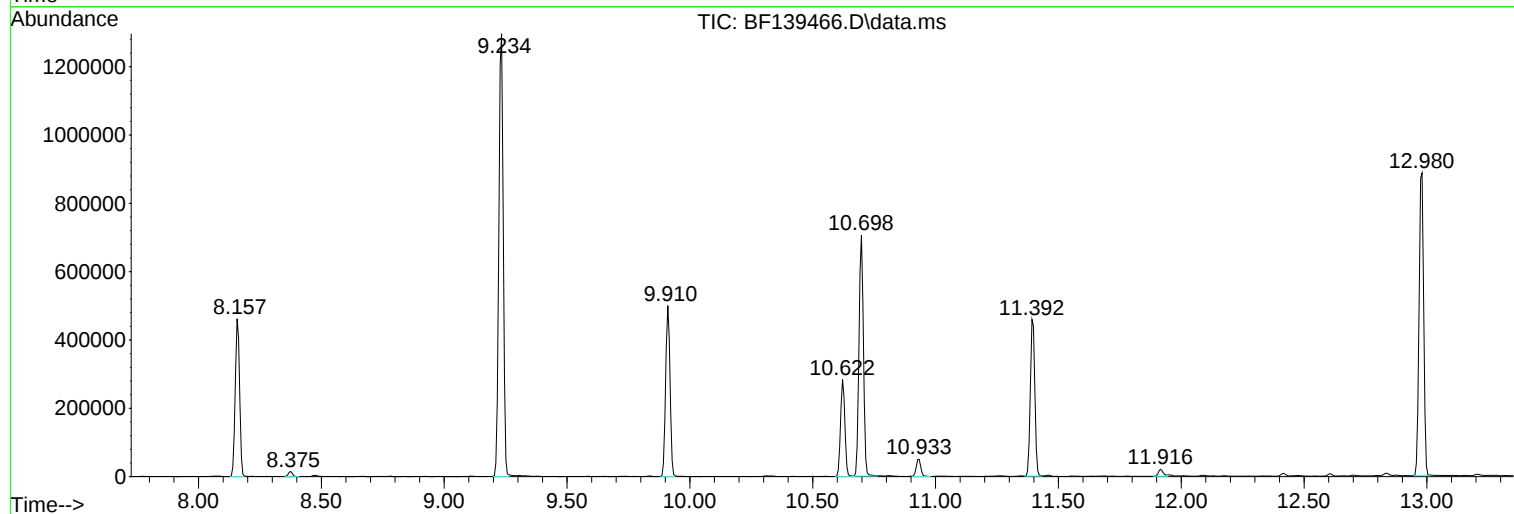
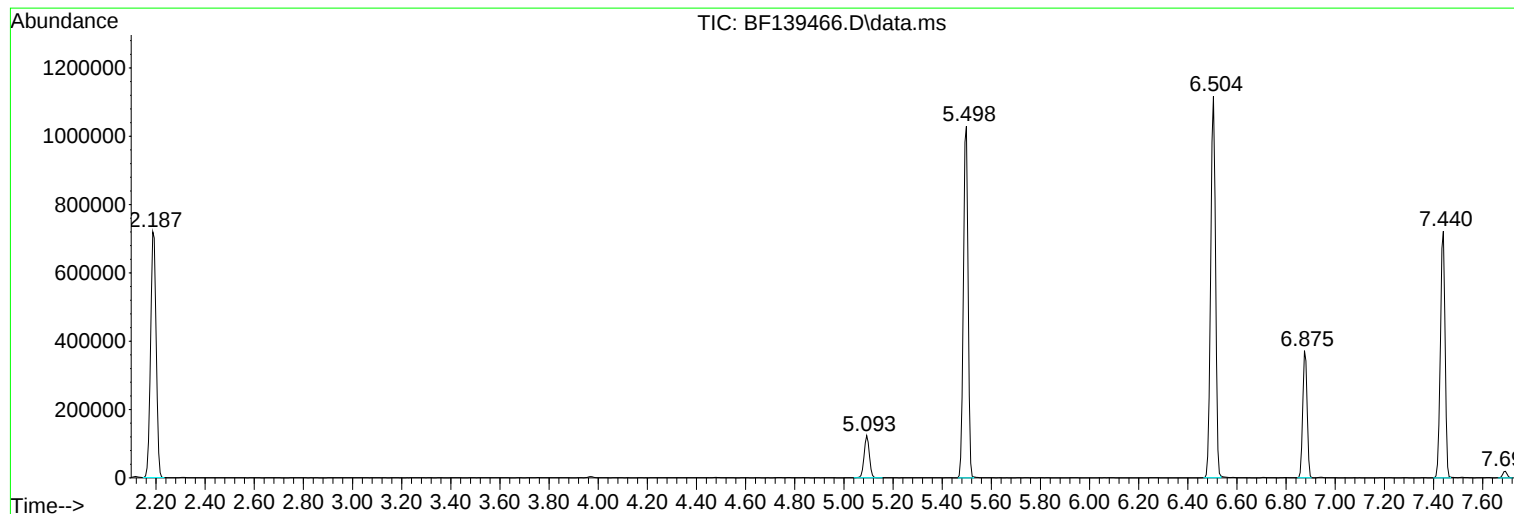
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF139466.D
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Instrument :
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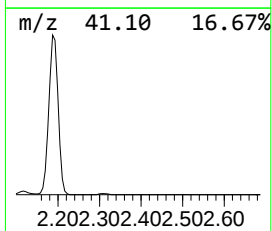
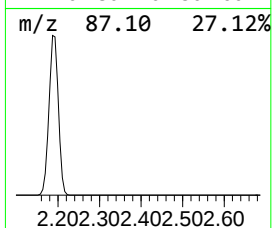
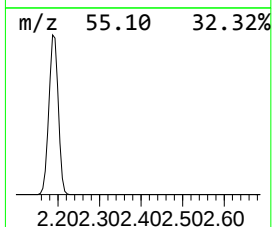
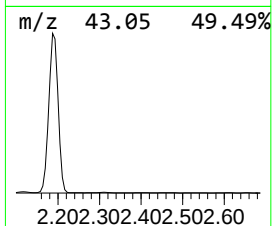
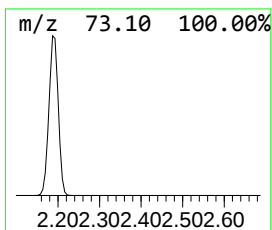
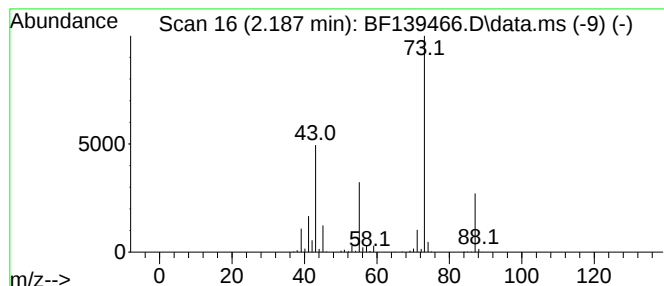
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.187	48.70 ng	1117290	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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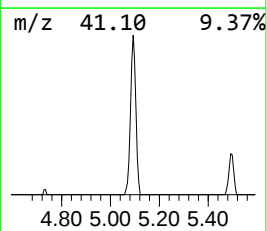
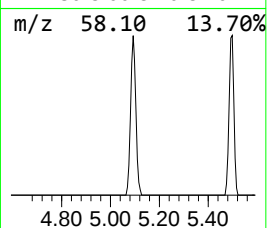
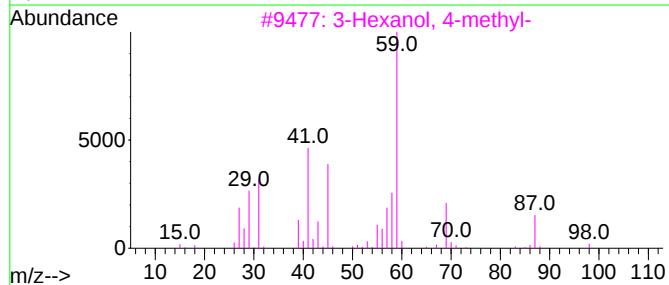
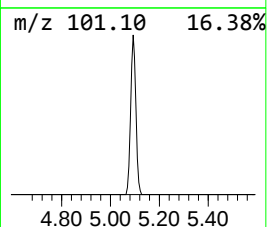
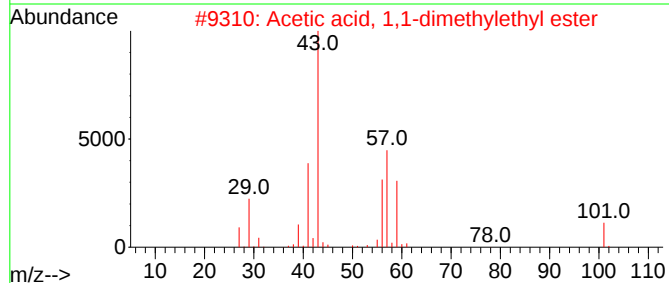
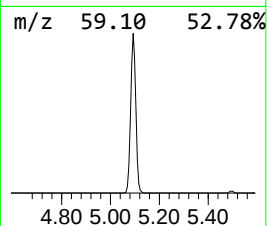
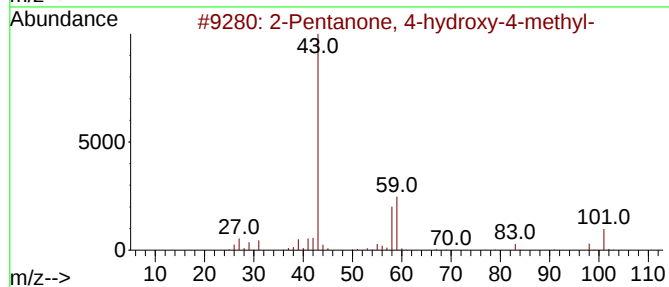
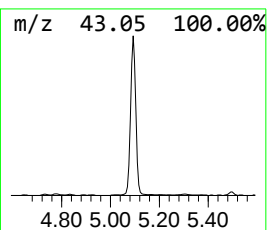
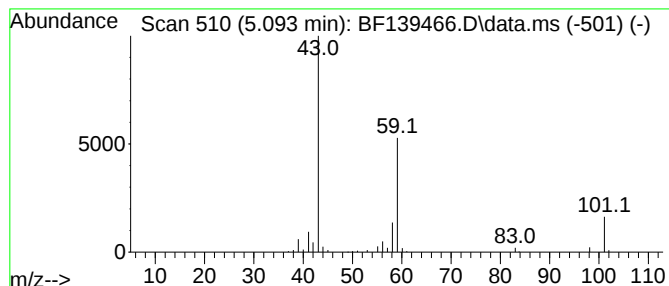
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	7.96 ng	182644	1,4-Dichlorobenzene-d4	6.875

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	38
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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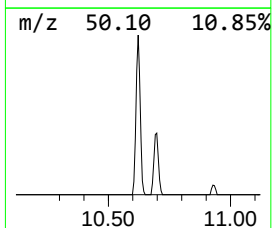
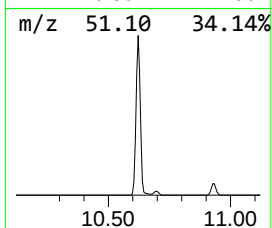
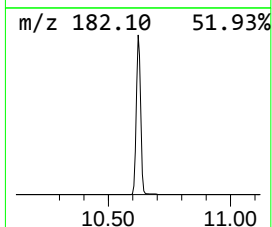
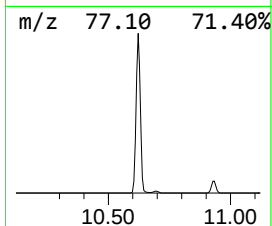
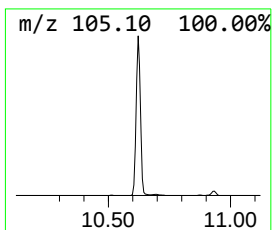
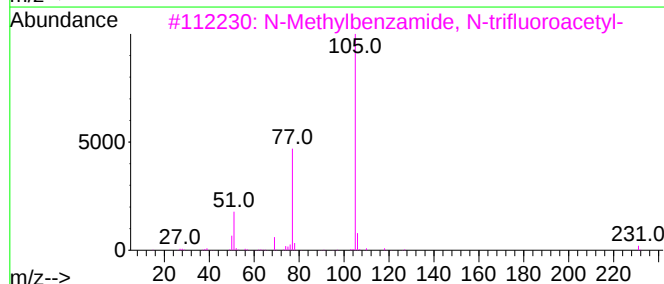
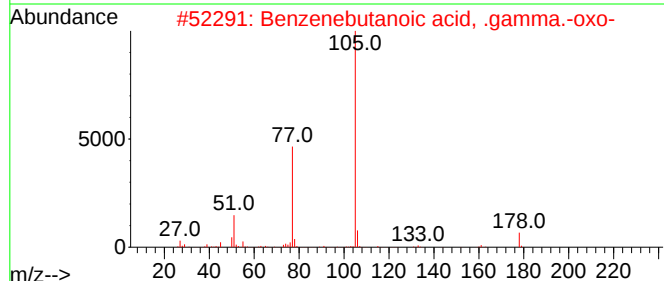
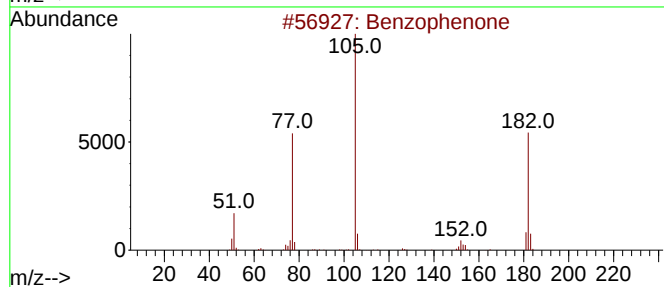
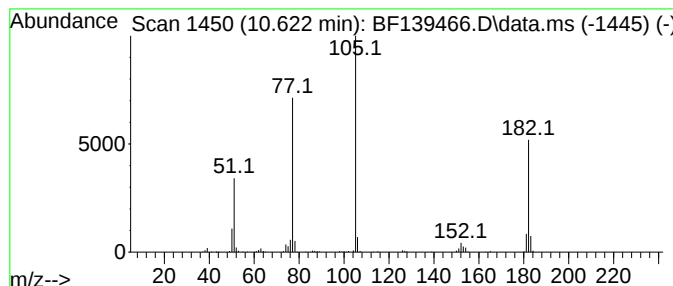
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	11.46 ng	346285	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50
4			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
5			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50



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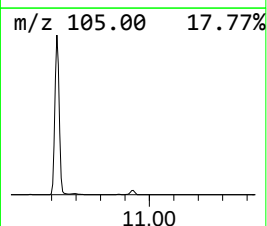
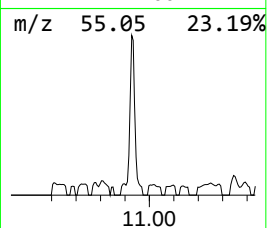
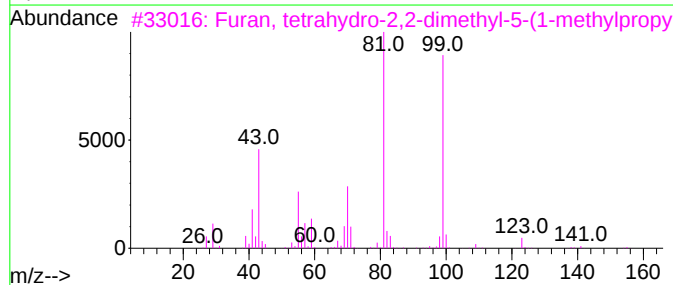
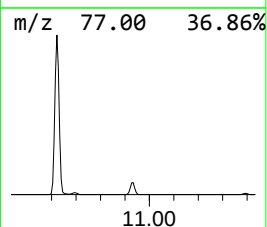
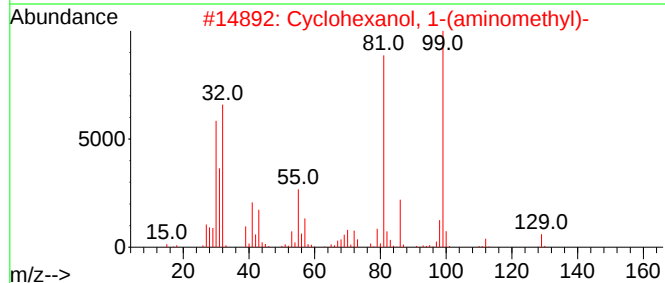
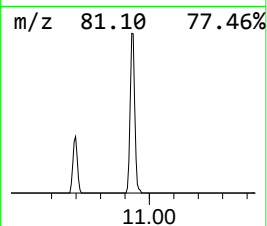
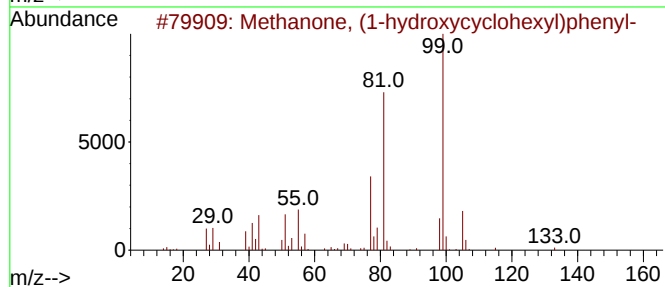
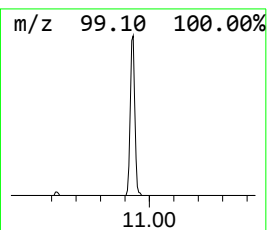
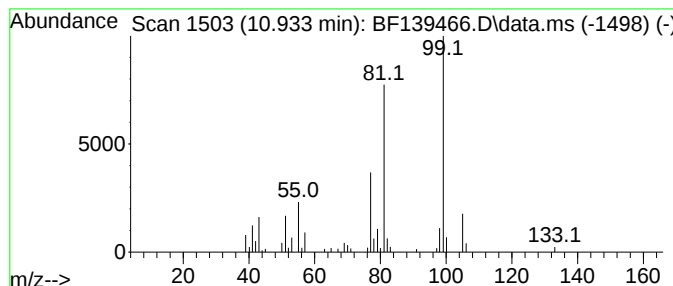
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.933	2.28 ng	66453	Phenanthrene-d10		11.392	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...		204	C13H16O2	000947-19-3	91
2	Cyclohexanol, 1-(aminomethyl)-		129	C7H15NO	004000-72-0	59
3	Furan, tetrahydro-2,2-dimethyl-5...		156	C10H20O	033978-70-0	53
4	1,1'-Bicyclohexyl-1,1'-diol		198	C12H22O2	002888-11-1	45
5	1-Hydroxycyclohexanecarboxylic acid		144	C7H12O3	001123-28-0	45



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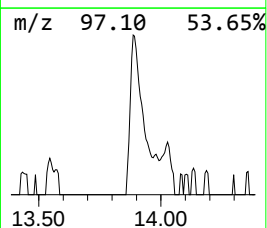
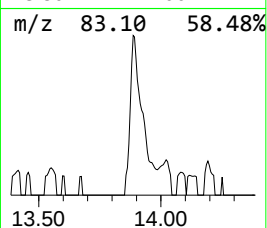
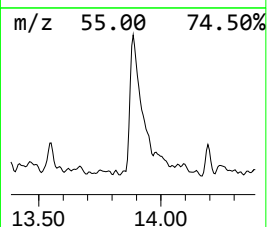
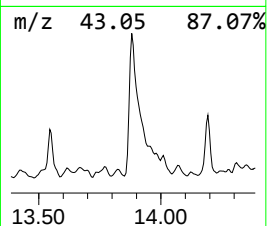
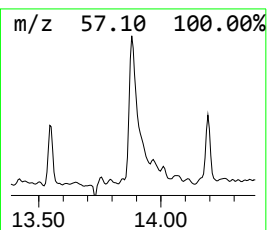
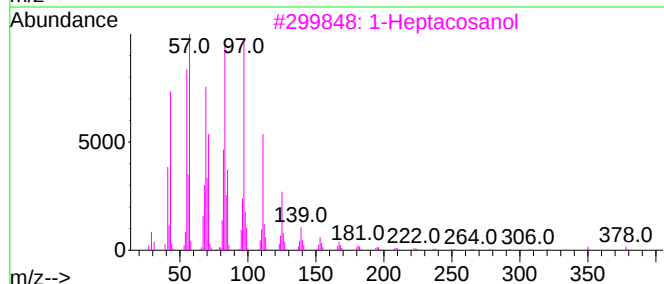
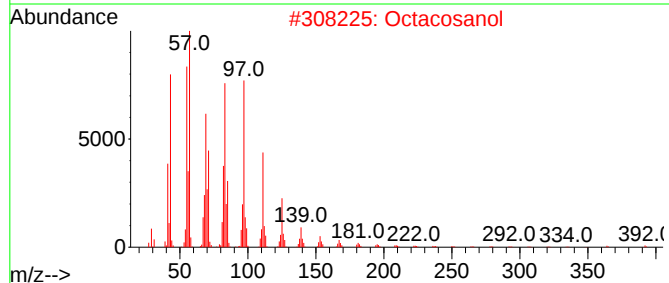
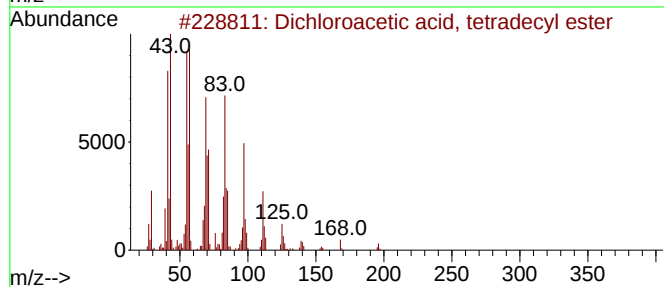
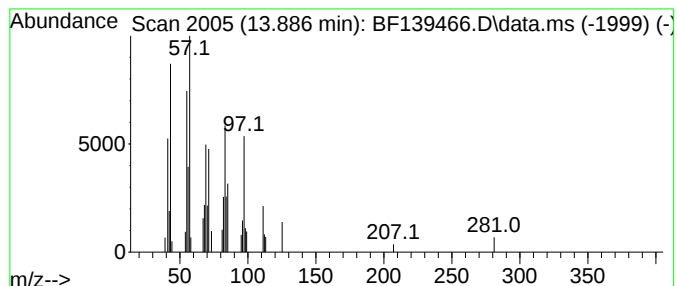
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Peak Number 5 Dichloroacetic acid, tetrad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.93 ng	61961	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	90
2			Octacosanol	410	C28H58O	000557-61-9	87
3			1-Heptacosanol	396	C27H56O	002004-39-9	87
4			17-Pentatriacontene	491	C35H70	006971-40-0	87
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	83



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.187	48.7	ng	1117290	1	6.875	458865	20.0
2-Pentanone, 4-...	5.093	8.0	ng	182644	1	6.875	458865	20.0
Benzophenone	10.622	11.5	ng	346285	3	9.910	604160	20.0
Methanone, (1-h...	10.933	2.3	ng	66453	4	11.392	582354	20.0
Dichloroacetic ...	13.886	3.9	ng	61961	5	14.027	315463	20.0