

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
 Data File : BF139030.D
 Acq On : 15 Aug 2024 19:11
 Operator : RC/JU
 Sample : P3580-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 923-K1-SD-0.5-1-081224

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-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139030.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	21	rVB	562913	671881	69.62%	9.539%
2	3.428	223	227	240	rBV2	3174	13051	1.35%	0.185%
3	5.063	500	505	524	rVB	36688	60767	6.30%	0.863%
4	5.469	569	574	601	rBV	658493	912089	94.51%	12.949%
5	6.481	741	746	767	rBV	711361	965079	100.00%	13.702%
6	6.834	802	806	814	rBB	184390	224121	23.22%	3.182%
7	7.398	897	902	917	rBV	434276	586337	60.76%	8.325%
8	7.663	943	947	953	rBV	9462	15736	1.63%	0.223%
9	8.116	1019	1024	1042	rVB	237856	295121	30.58%	4.190%
10	8.433	1074	1078	1091	rBV	31234	50045	5.19%	0.711%
11	9.186	1201	1206	1211	rBV	751960	914781	94.79%	12.988%
12	9.869	1317	1322	1330	rVB	251646	329594	34.15%	4.679%
13	9.957	1332	1337	1344	rVV	20478	30063	3.12%	0.427%
14	10.657	1451	1456	1470	rBV	449647	581653	60.27%	8.258%
15	11.357	1569	1575	1584	rBV	240512	315461	32.69%	4.479%
16	11.874	1659	1663	1678	rVB5	6937	14719	1.53%	0.209%
17	12.798	1816	1820	1828	rVB3	7559	11257	1.17%	0.160%
18	12.933	1838	1843	1848	rBV	513817	620491	64.29%	8.809%
19	13.210	1886	1890	1897	rVB	38186	44064	4.57%	0.626%
20	13.827	1989	1995	2009	rBV4	15049	45052	4.67%	0.640%
21	13.998	2019	2024	2034	rVB	128150	166486	17.25%	2.364%
22	15.462	2267	2273	2285	rVB	111914	175586	18.19%	2.493%

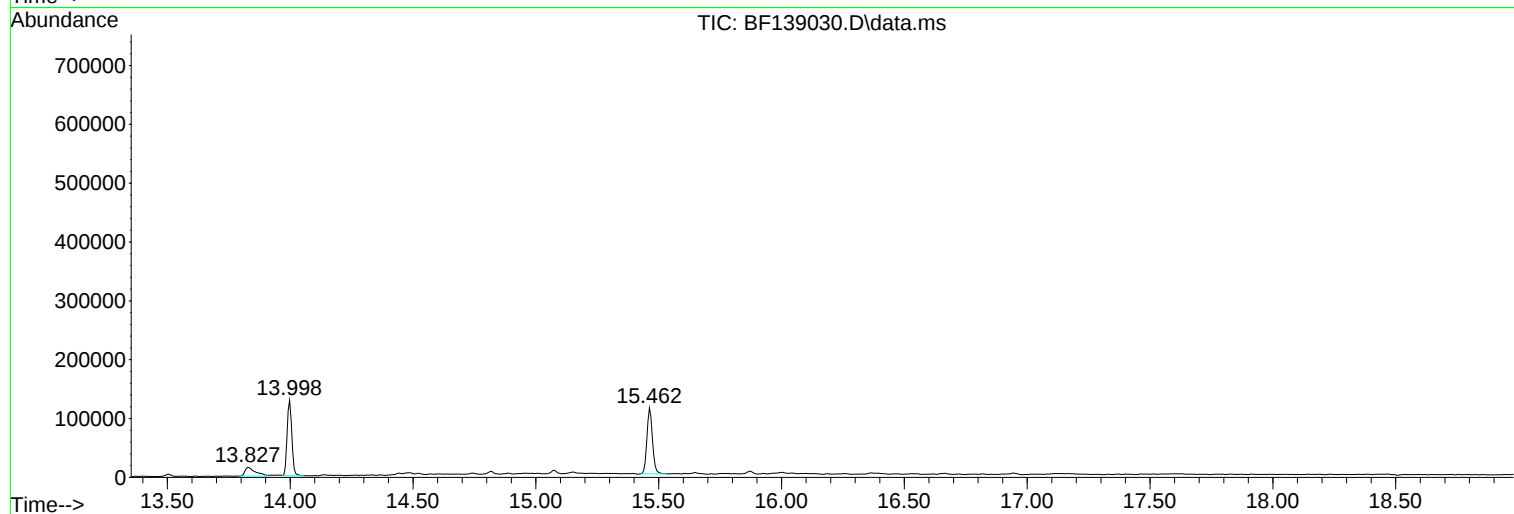
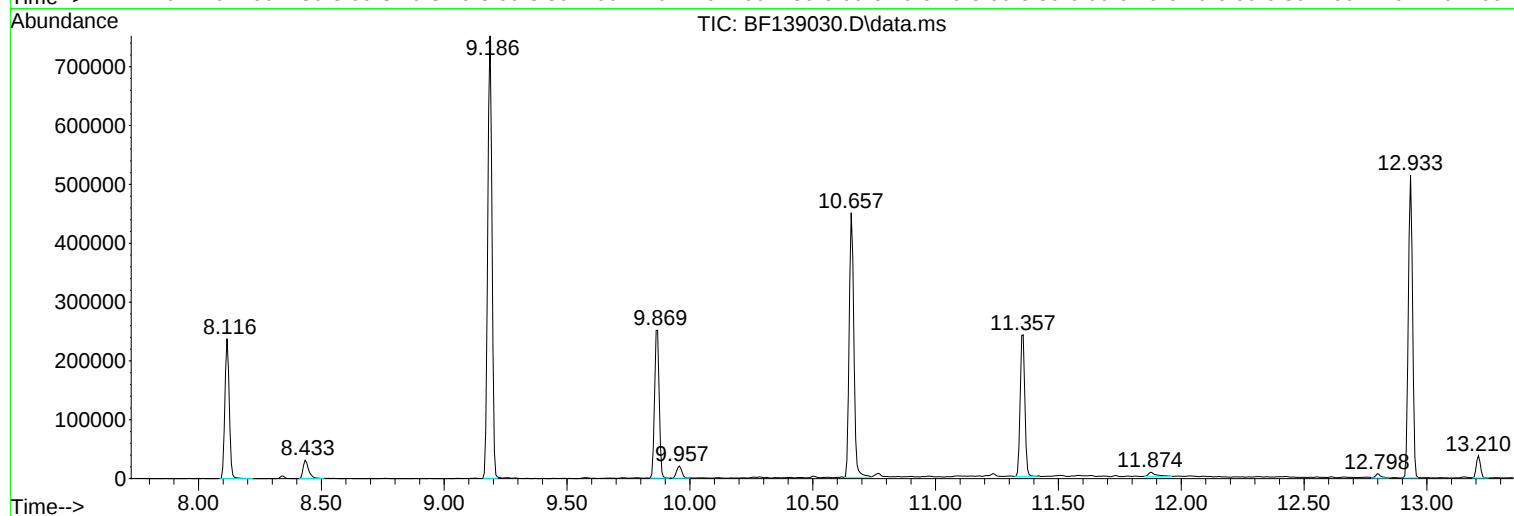
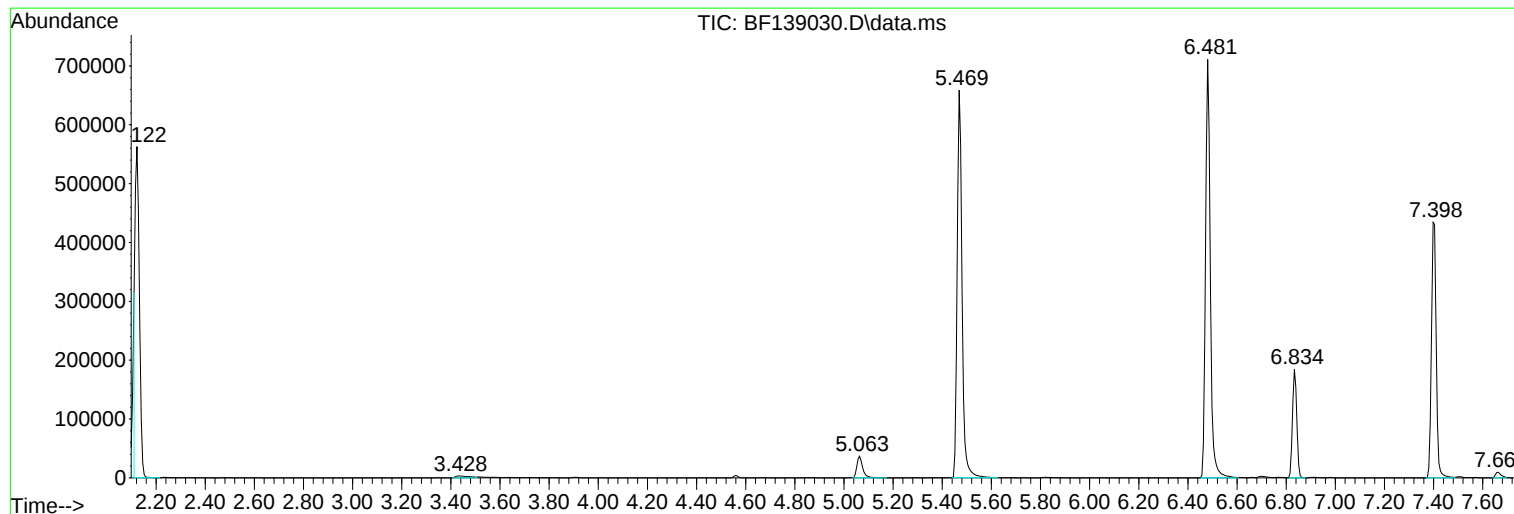
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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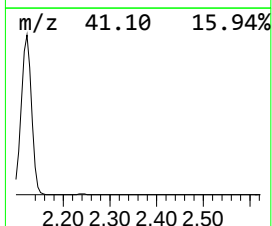
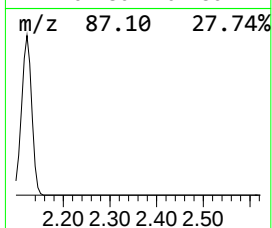
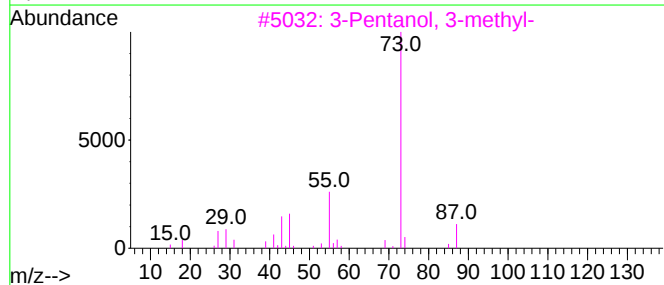
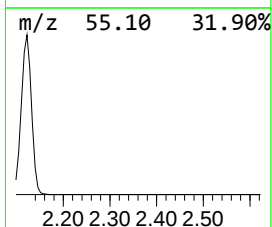
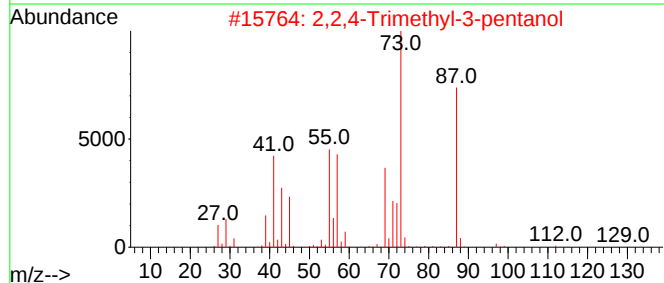
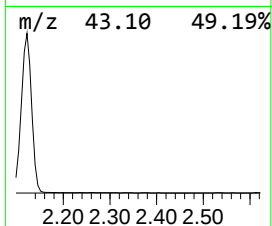
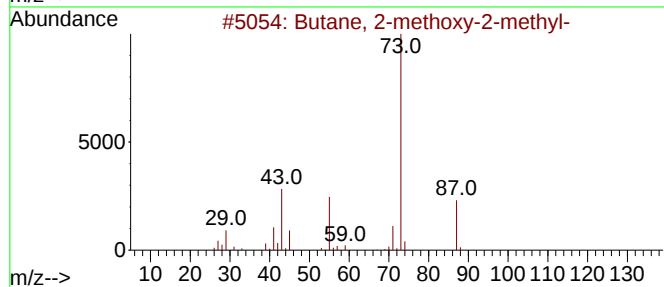
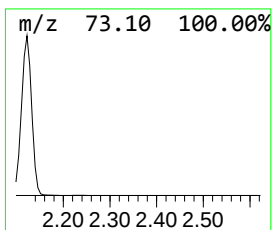
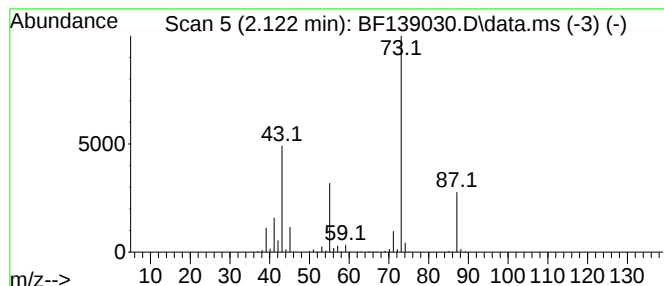
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.122	59.96 ng	671881	1,4-Dichlorobenzene-d4	6.834

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	39
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
4			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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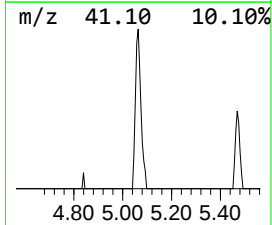
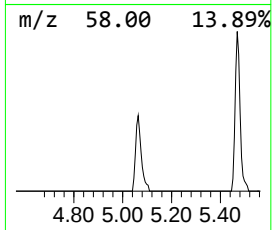
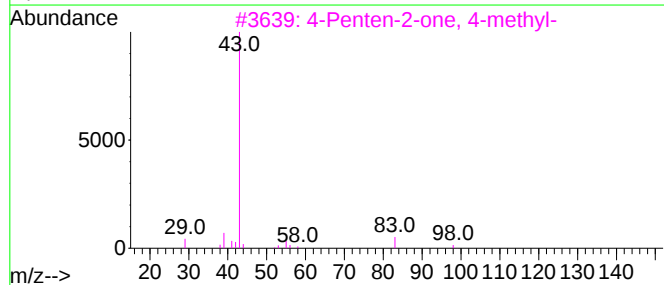
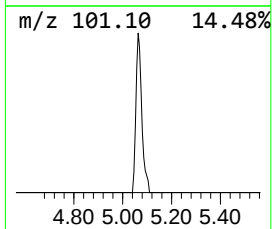
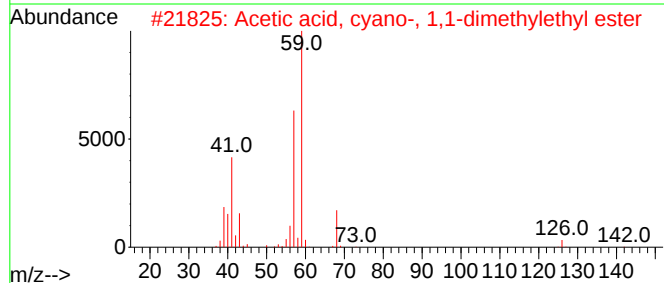
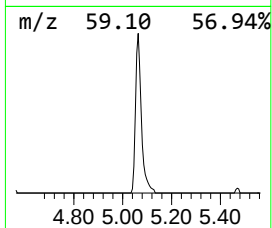
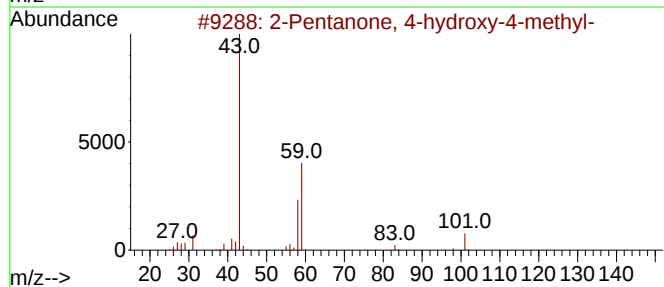
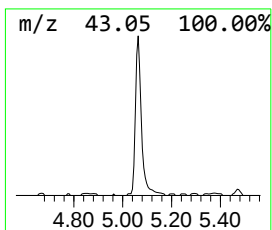
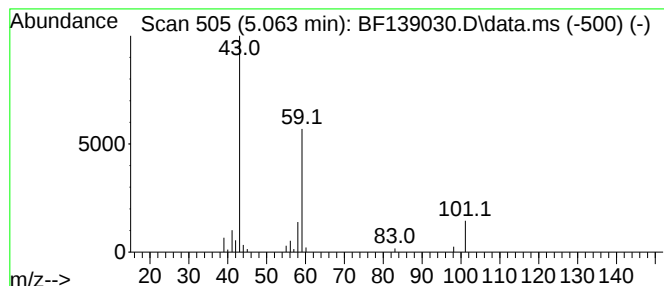
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	5.42 ng	60767	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9		
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9		



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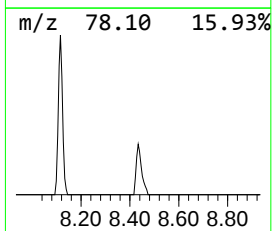
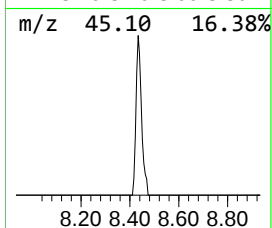
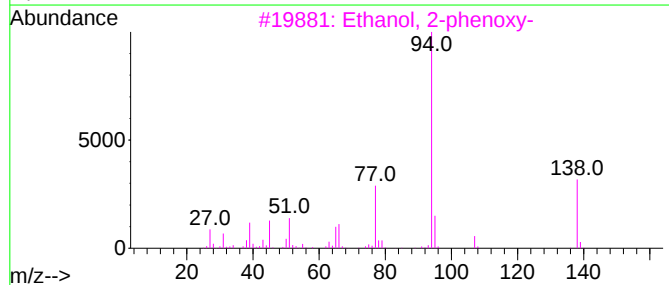
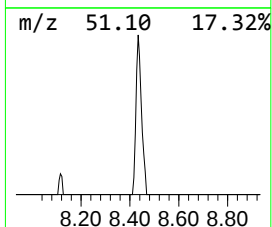
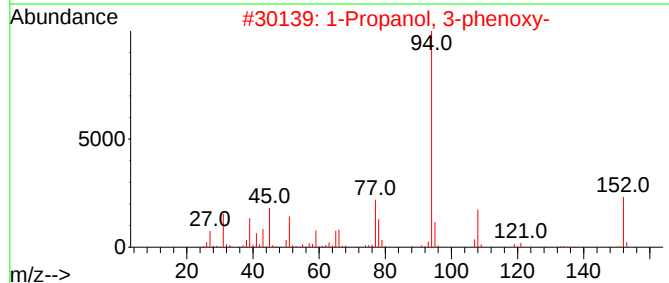
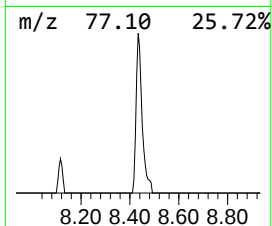
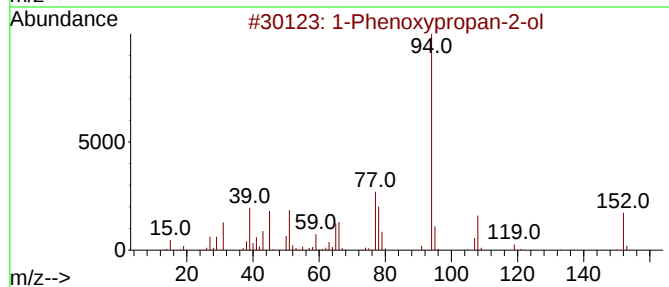
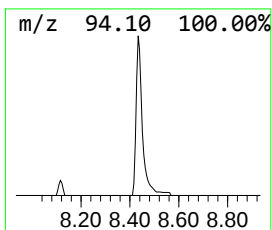
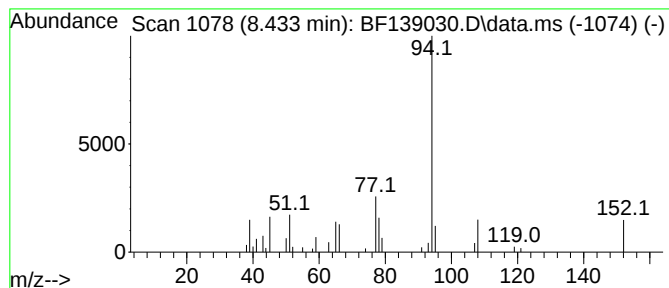
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	3.39 ng	50045	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	45



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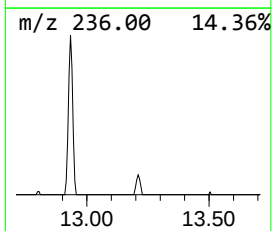
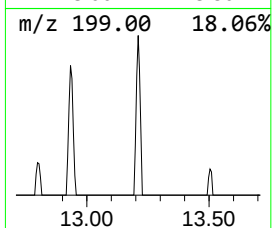
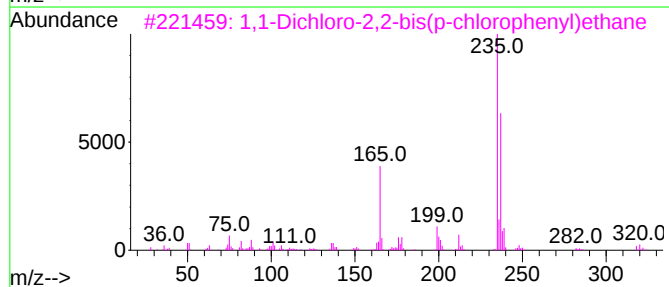
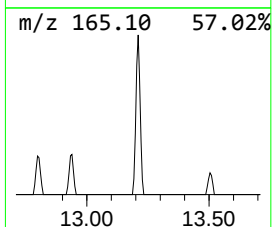
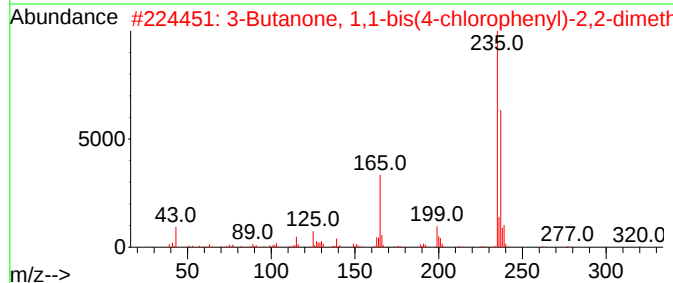
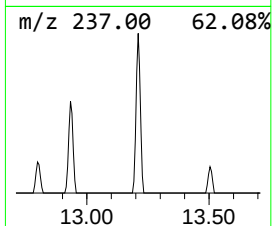
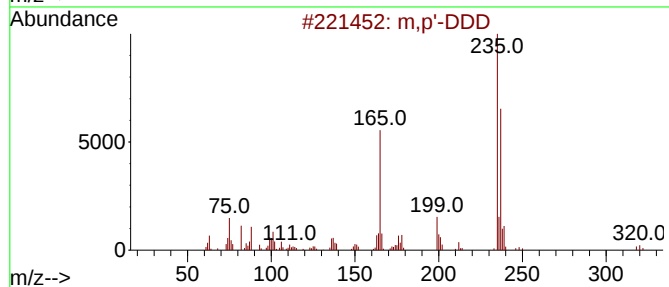
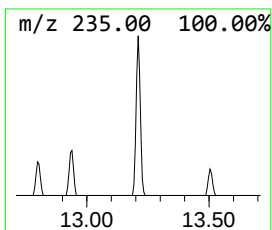
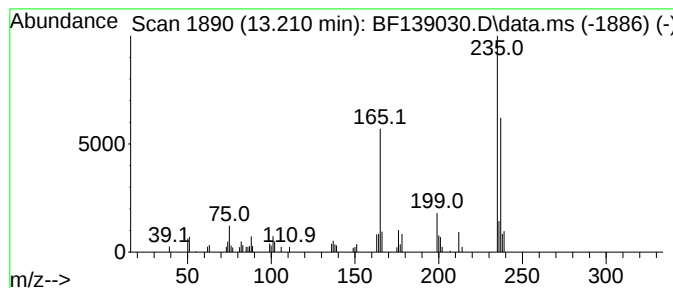
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 m,p'-DDD Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.210	5.29 ng	44064	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	m,p'-DDD			318	C14H10Cl4	004329-12-8	91
2	3-Butanone, 1,1-bis(4-chlorophen...			320	C18H18Cl2O	1000158-20-4	86
3	1,1-Dichloro-2,2-bis(p-chlorophe...			318	C14H10Cl4	000072-54-8	80
4	Mitotane			318	C14H10Cl4	000053-19-0	53
5	(1Z)-1-(3-Ethyl-5-hydroxy-2(3H)-...			235	C12H13NO2S	1169755-45-6	50



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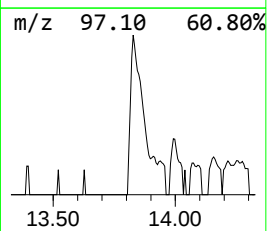
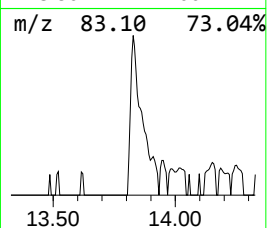
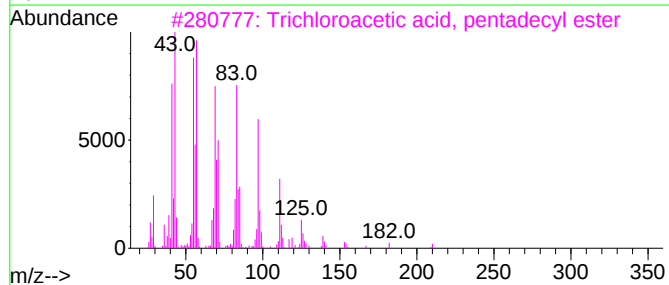
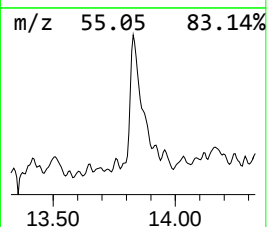
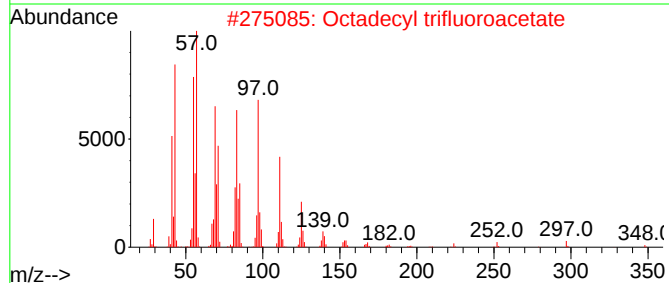
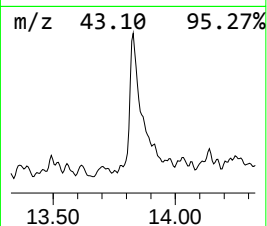
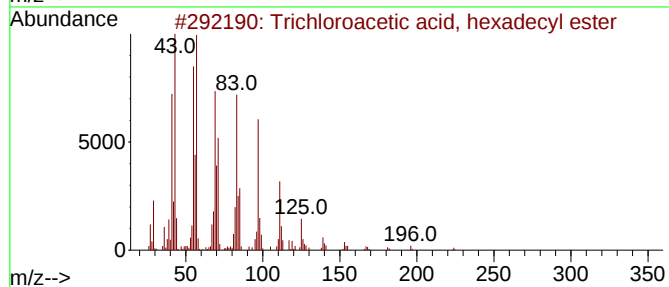
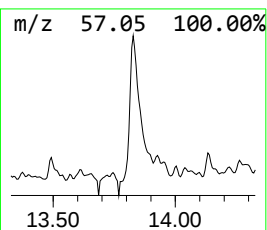
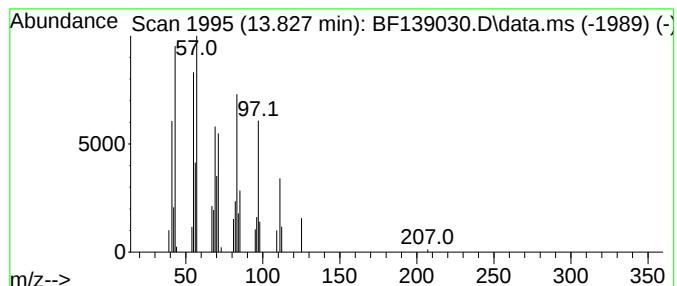
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	5.41 ng	45052	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4			Octacosanol	410	C28H58O	000557-61-9	91
5			17-Pentatriacontene	491	C35H70	006971-40-0	87



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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
Butane, 2-metho...	2.122	60.0	ng	671881	1	6.834	224121	20.0
2-Pentanone, 4-...	5.063	5.4	ng	60767	1	6.834	224121	20.0
1-Phenoxypropan...	8.433	3.4	ng	50045	2	8.116	295121	20.0
m,p'-DDD	13.210	5.3	ng	44064	5	13.998	166486	20.0
Trichloroacetic...	13.827	5.4	ng	45052	5	13.998	166486	20.0