

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102124\
 Data File : BF139896.D
 Acq On : 21 Oct 2024 11:55
 Operator : RC/JU
 Sample : P4425-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-5

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139896.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	9	17	32	rVB	1855565	3043186	88.79%	11.135%
2	5.110	505	513	524	rVB	187726	279119	8.14%	1.021%
3	5.504	573	580	585	rBV	2224443	2954457	86.20%	10.811%
4	6.504	743	750	755	rBV	2269940	3145470	91.77%	11.510%
5	6.887	810	815	821	rBV	800434	1007674	29.40%	3.687%
6	7.445	904	910	915	rBV	1531071	1975267	57.63%	7.228%
7	7.698	948	953	960	rBV	106392	128382	3.75%	0.470%
8	8.169	1027	1033	1038	rBV	1064698	1321047	38.54%	4.834%
9	8.381	1063	1069	1077	rVB	36478	50863	1.48%	0.186%
10	9.245	1210	1216	1221	rBV	2683068	3427575	100.00%	12.542%
11	9.922	1326	1331	1337	rBV	1156704	1479530	43.17%	5.414%
12	10.633	1447	1452	1459	rBV	286424	367434	10.72%	1.344%
13	10.710	1459	1465	1482	rVV	1511668	1908193	55.67%	6.982%
14	11.410	1579	1584	1589	rBV	1151479	1403570	40.95%	5.136%
15	11.480	1591	1596	1599	rVB2	31393	38281	1.12%	0.140%
16	11.933	1667	1673	1686	rBV2	110655	185884	5.42%	0.680%
17	12.716	1802	1806	1815	rBV	21908	36511	1.07%	0.134%
18	12.998	1848	1854	1859	rBV	2120608	2724983	79.50%	9.971%
19	13.892	2001	2006	2017	rBV	96303	172184	5.02%	0.630%
20	14.051	2027	2033	2041	rBV	593432	797786	23.28%	2.919%
21	15.527	2278	2284	2298	rVB	574081	881918	25.73%	3.227%

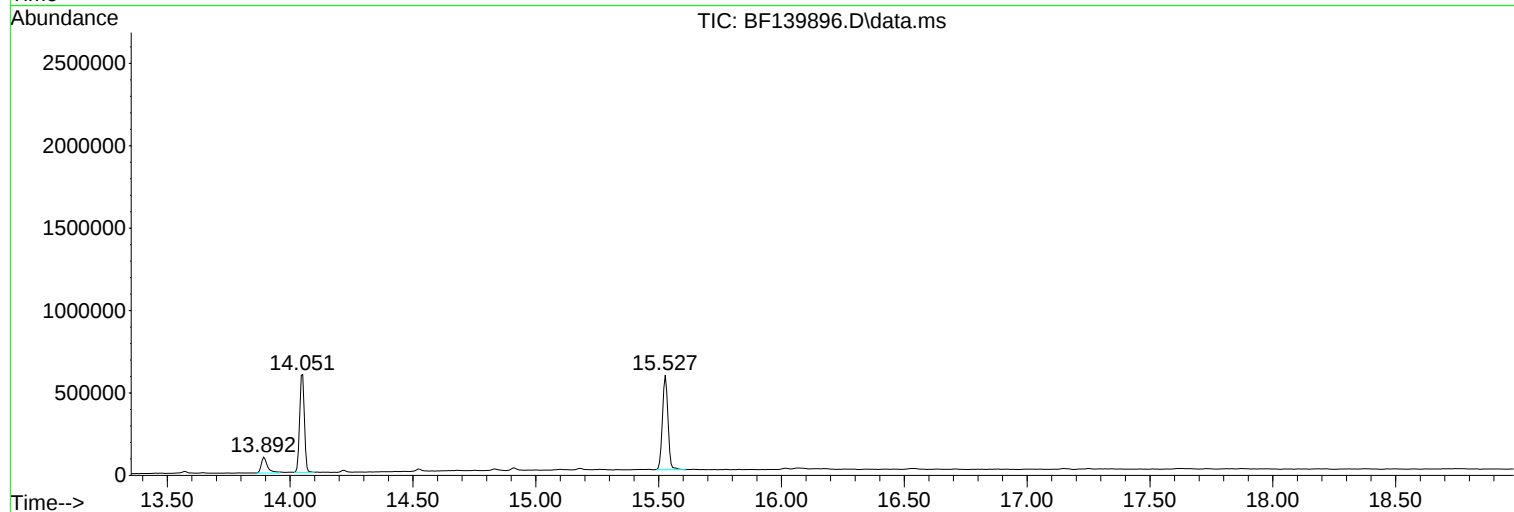
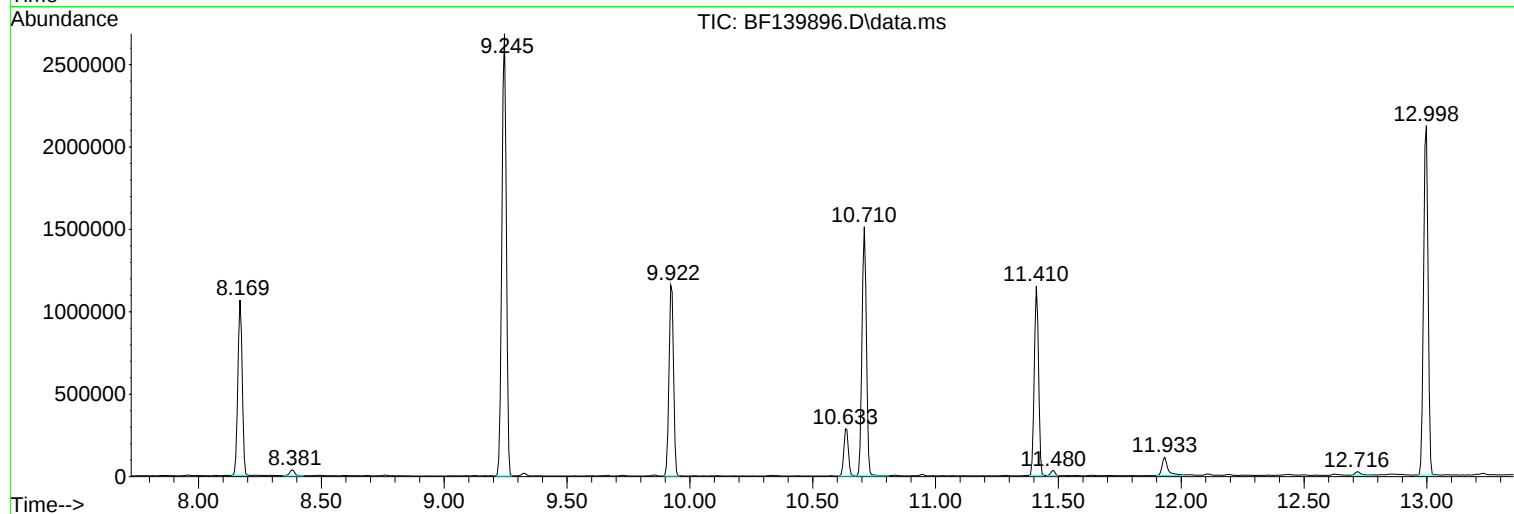
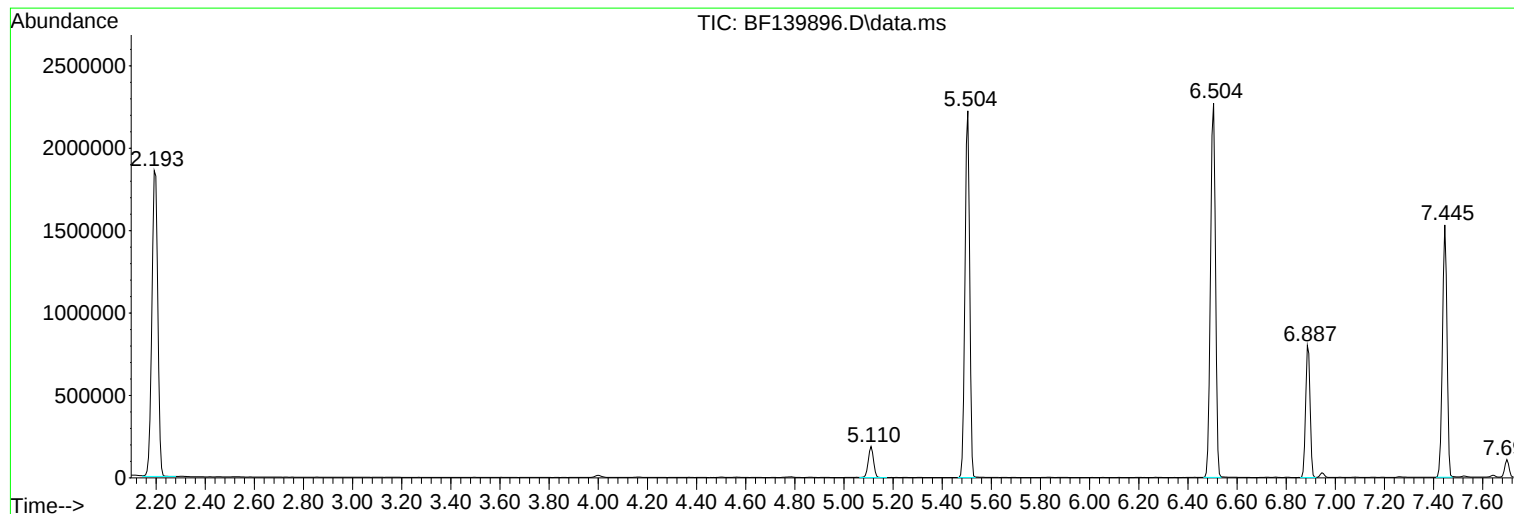
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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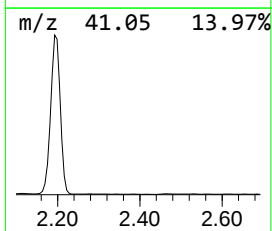
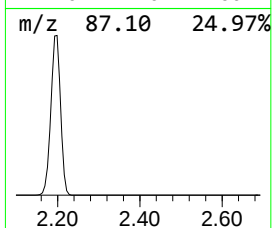
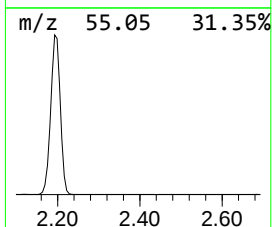
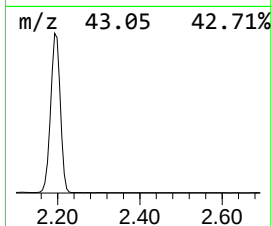
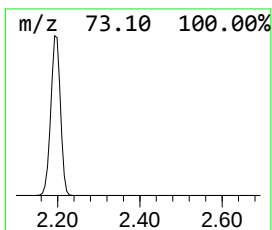
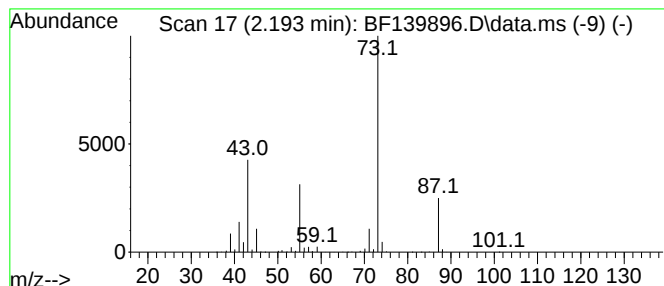
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	60.40 ng	3043190	1,4-Dichlorobenzene-d4	6.887

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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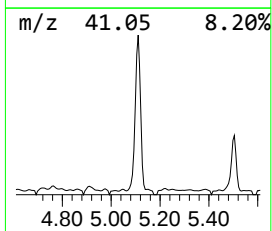
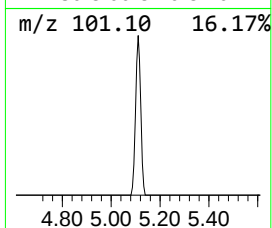
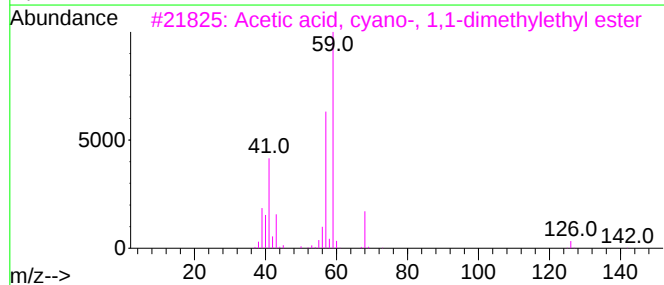
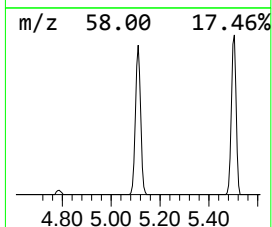
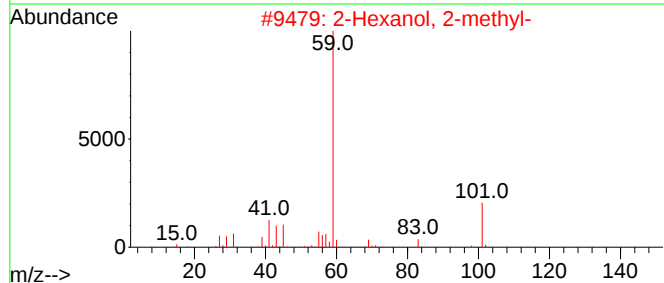
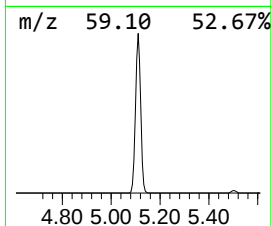
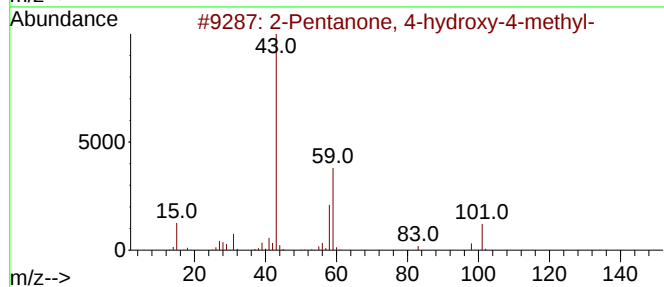
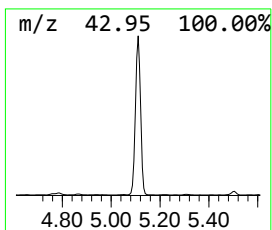
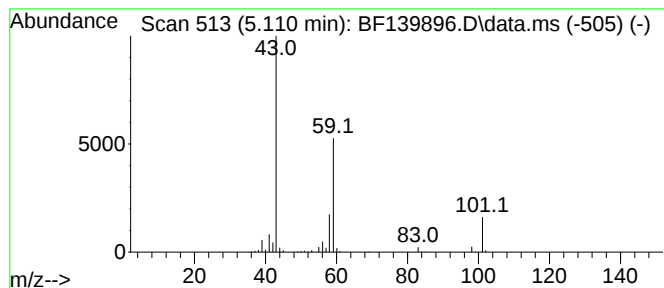
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.54 ng	279119	1,4-Dichlorobenzene-d4	6.887

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			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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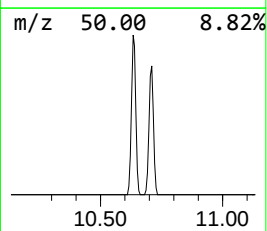
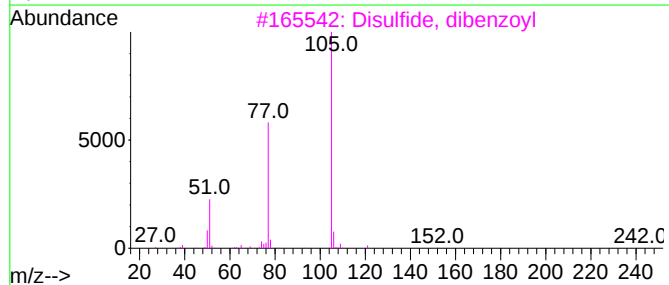
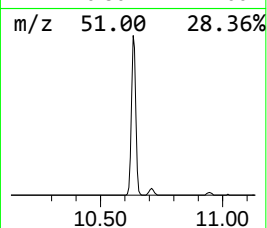
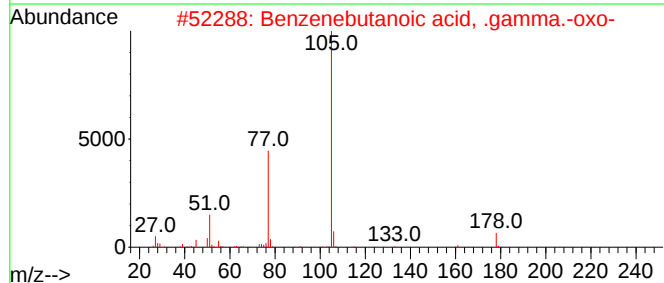
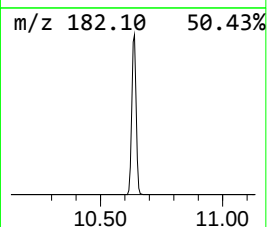
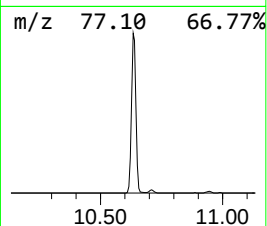
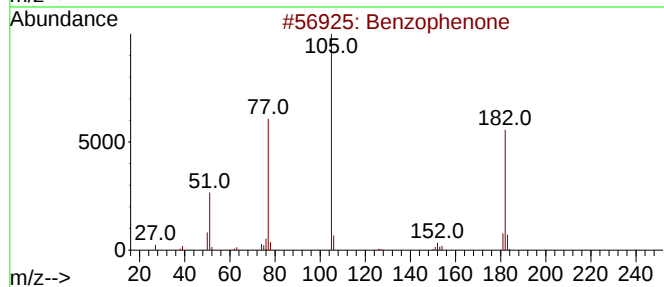
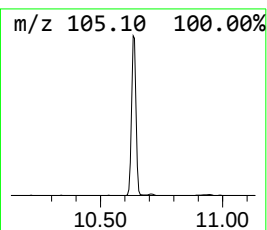
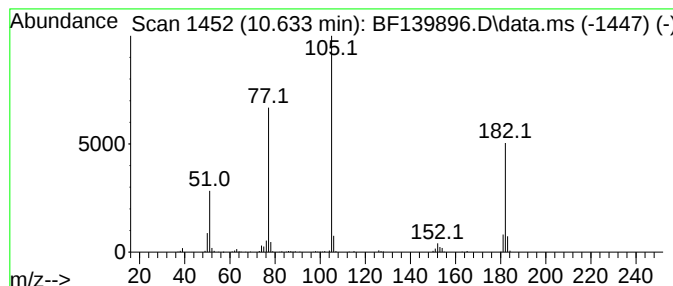
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	4.97 ng	367434	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
3			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



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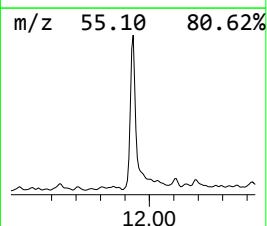
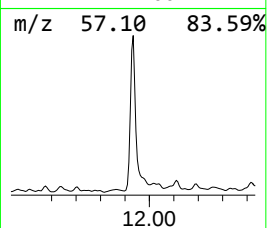
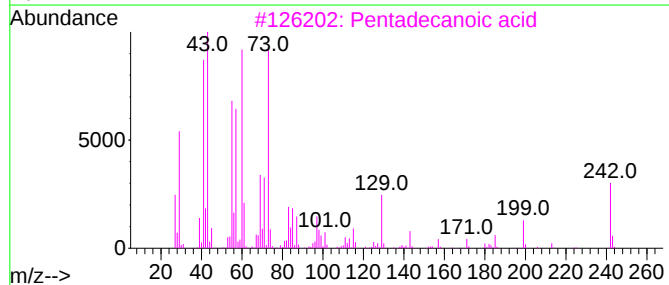
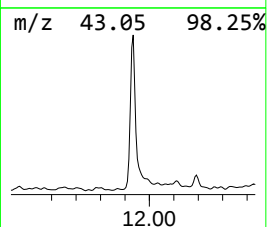
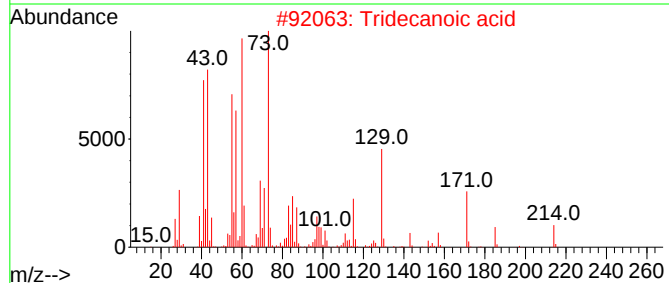
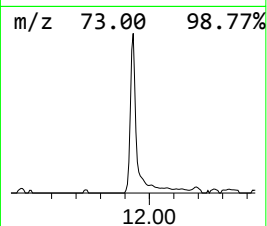
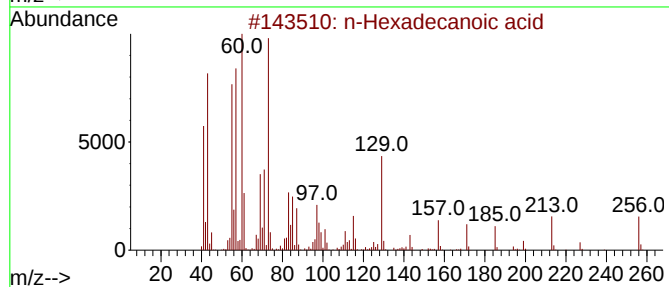
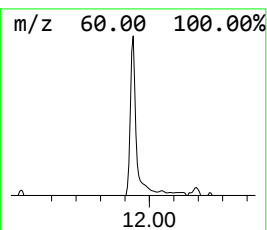
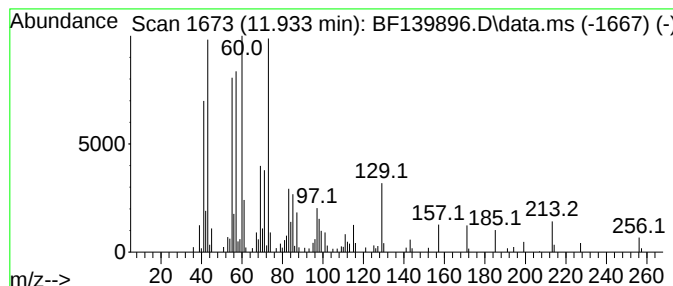
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.65 ng	185884	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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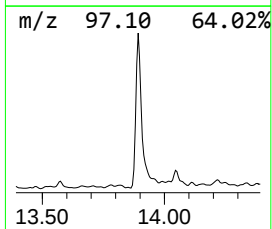
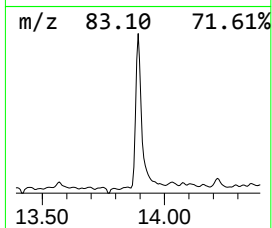
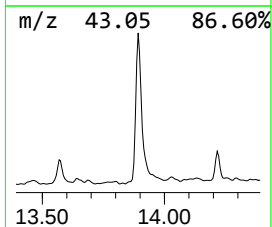
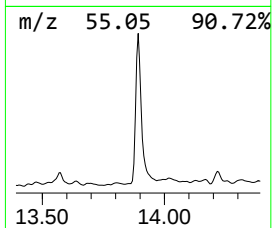
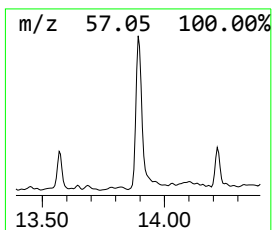
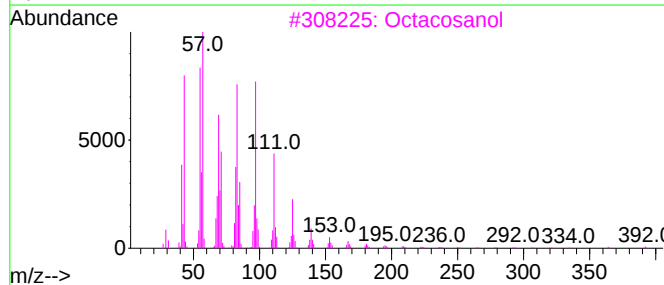
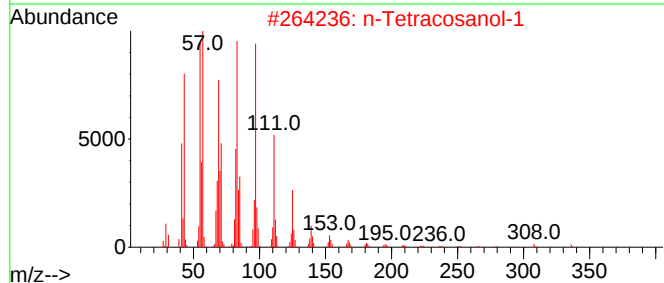
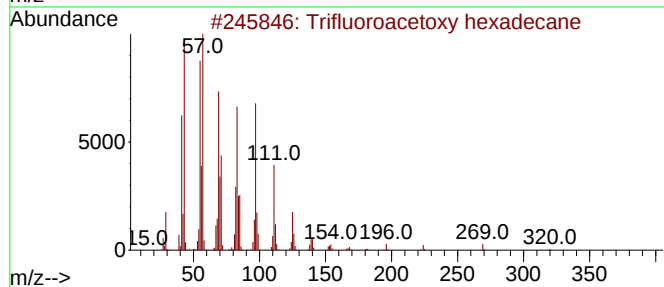
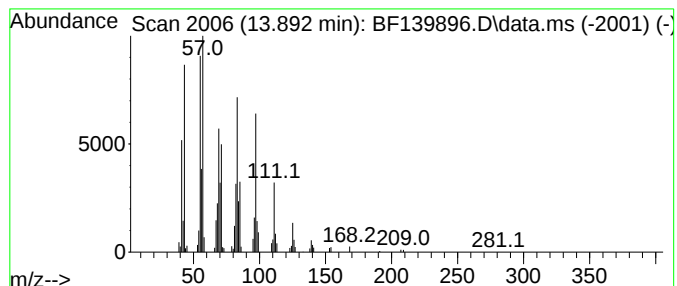
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.32 ng	172184	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			Octacosanol	410	C28H58O	000557-61-9	91
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			1-Docosene	308	C22H44	001599-67-3	91



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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...	2.193	60.4	ng	3043190	1	6.887	1007670	20.0
2-Pentanone, 4-...	5.110	5.5	ng	279119	1	6.887	1007670	20.0
Benzophenone	10.633	5.0	ng	367434	3	9.922	1479530	20.0
n-Hexadecanoic ...	11.933	2.6	ng	185884	4	11.410	1403570	20.0
Trifluoroacetox...	13.892	4.3	ng	172184	5	14.051	797786	20.0