

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091924\
 Data File : BF139470.D
 Acq On : 19 Sep 2024 18:23
 Operator : RC/JU
 Sample : P4015-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-1-TANK17

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: BF139470.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	12	22	30	rVB	1252322	1993913	65.66%	10.275%
2	5.110	504	513	525	rVB	113005	193585	6.38%	0.998%
3	5.504	573	580	585	rBV	1857752	2561310	84.35%	13.199%
4	6.510	744	751	756	rBV	1732905	2667749	87.85%	13.748%
5	6.875	808	813	818	rVB	427582	520206	17.13%	2.681%
6	7.440	902	909	914	rBV	1286228	1757777	57.89%	9.059%
7	7.687	947	951	957	rVB	38123	47147	1.55%	0.243%
8	8.157	1025	1031	1036	rBV	520331	646852	21.30%	3.333%
9	9.234	1207	1214	1219	rBV	2371685	3036551	100.00%	15.649%
10	9.910	1324	1329	1334	rBV	567328	693850	22.85%	3.576%
11	10.622	1445	1450	1457	rBV	183926	229370	7.55%	1.182%
12	10.698	1457	1463	1477	rBV	1294253	1669081	54.97%	8.601%
13	11.398	1576	1582	1587	rBV	474970	614654	20.24%	3.168%
14	11.916	1665	1670	1674	rBV	104164	146377	4.82%	0.754%
15	12.980	1845	1851	1856	rBV	1467078	1837252	60.50%	9.468%
16	13.892	1999	2006	2024	rBV2	29409	98578	3.25%	0.508%
17	14.027	2024	2029	2042	rVB	257102	335758	11.06%	1.730%
18	15.498	2273	2279	2291	rBV	229528	354629	11.68%	1.828%

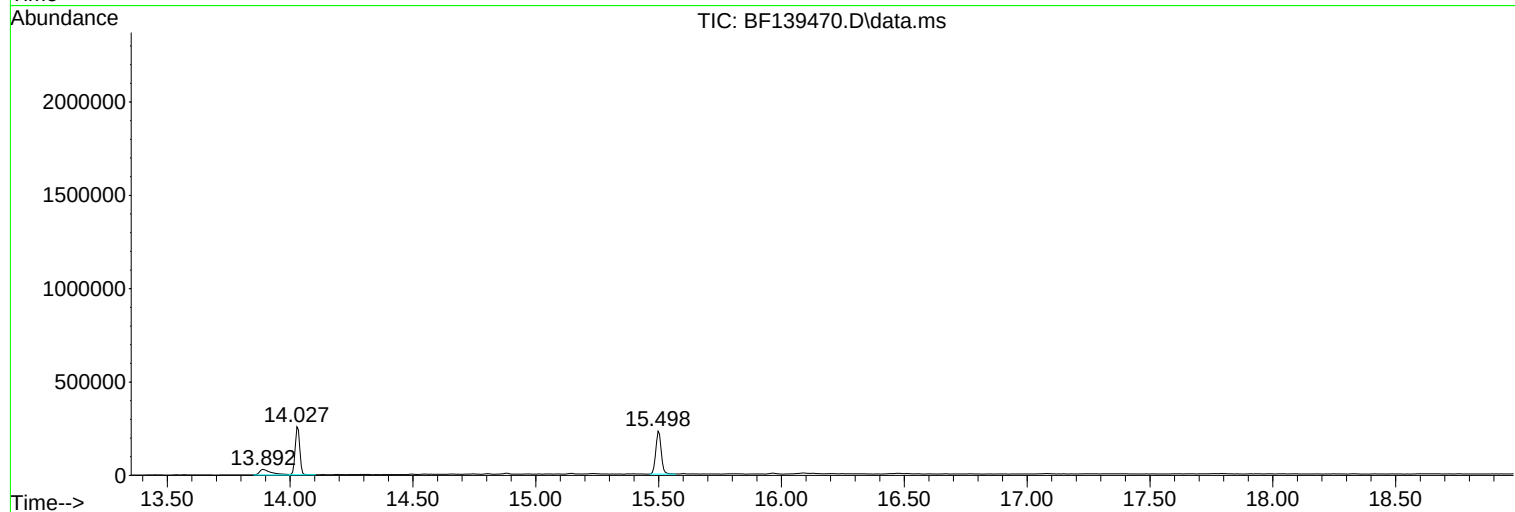
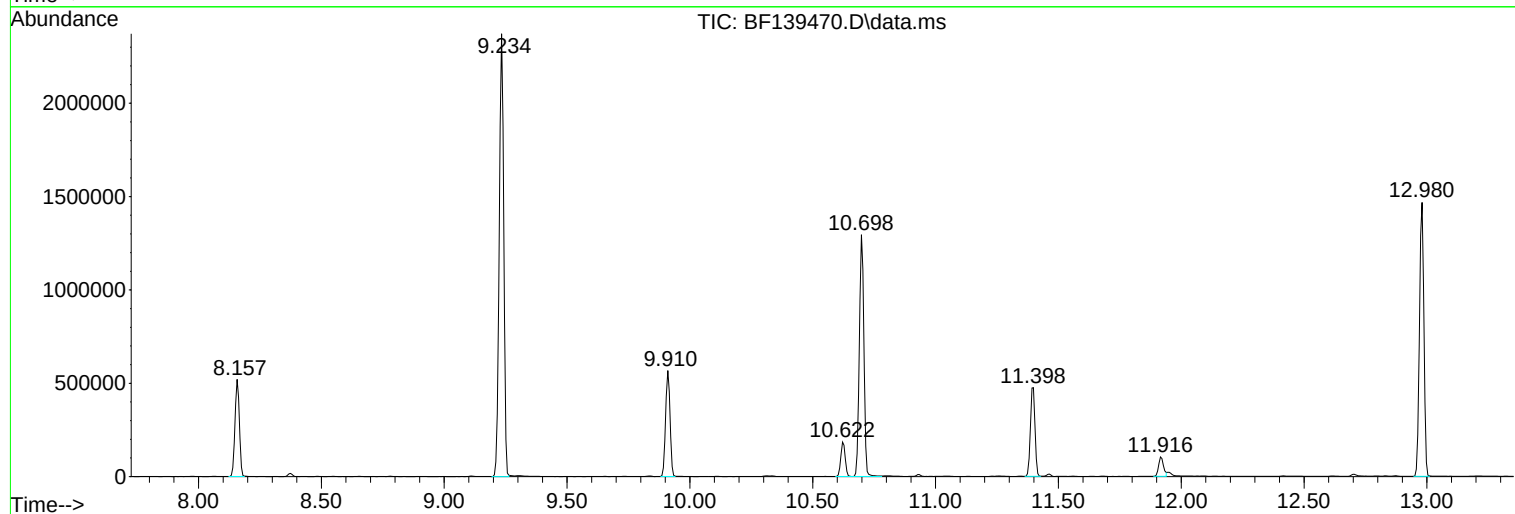
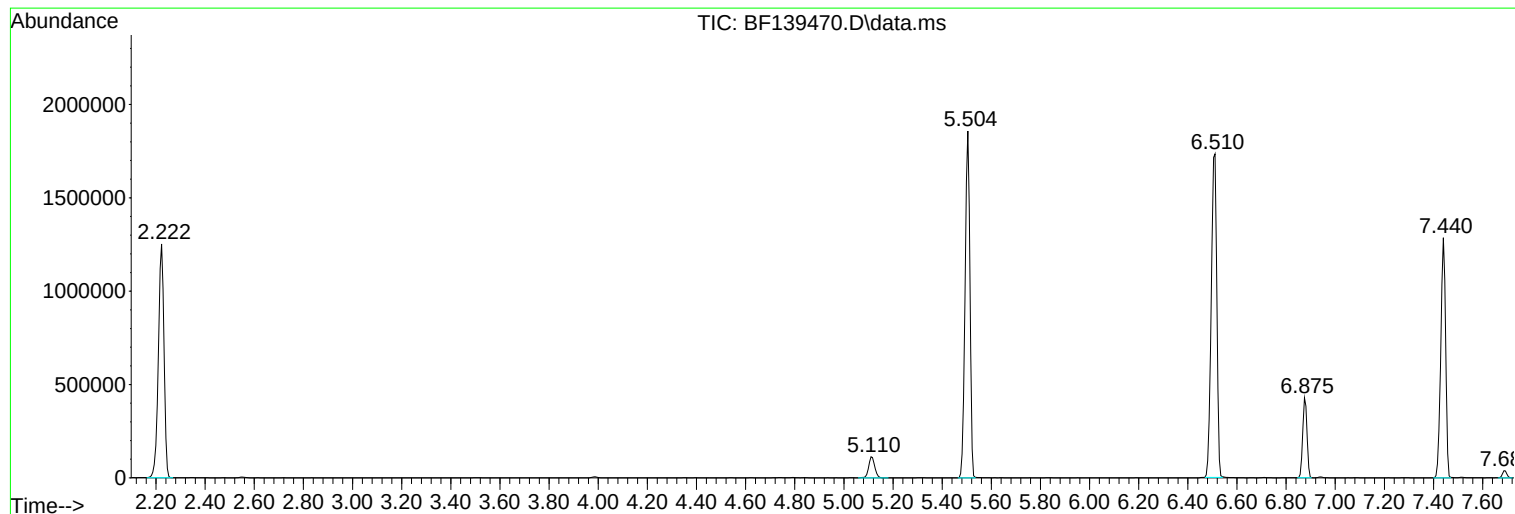
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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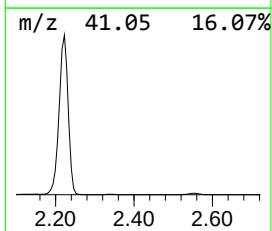
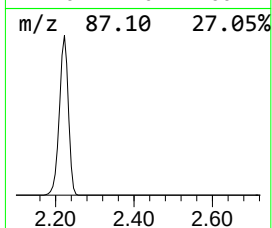
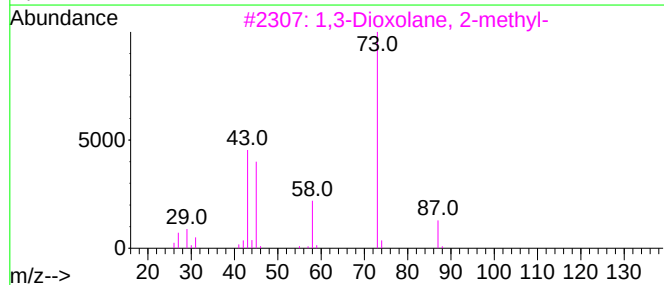
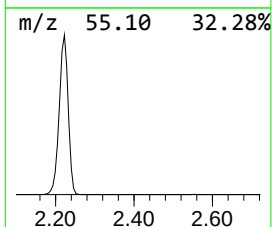
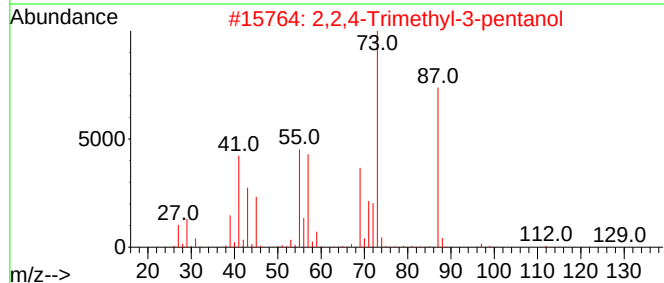
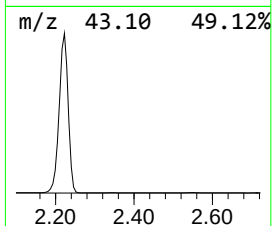
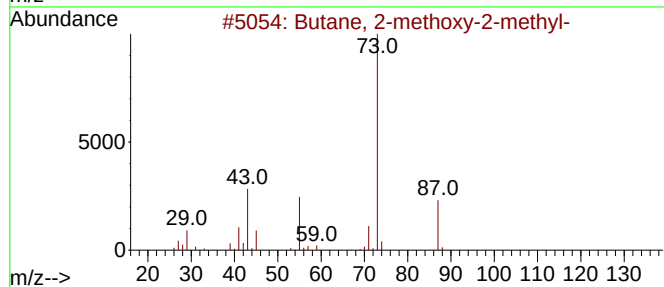
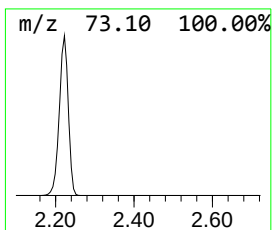
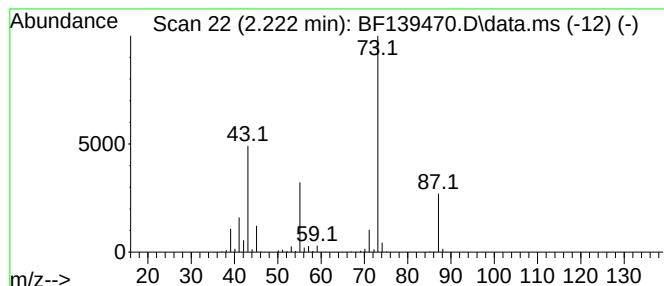
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.222	76.66 ng	1993910	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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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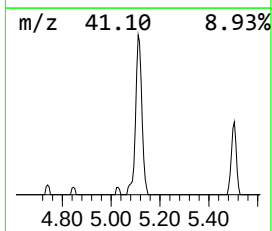
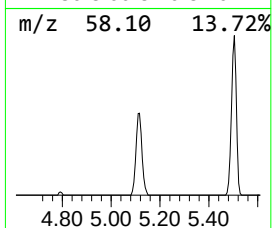
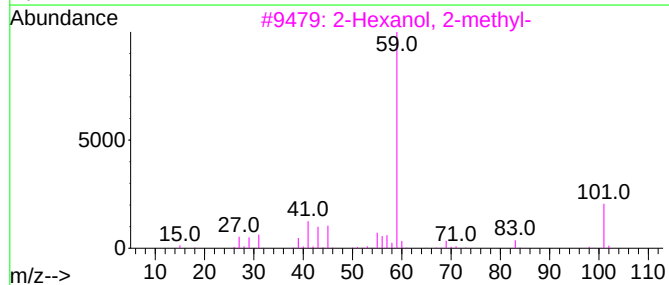
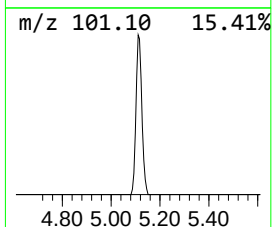
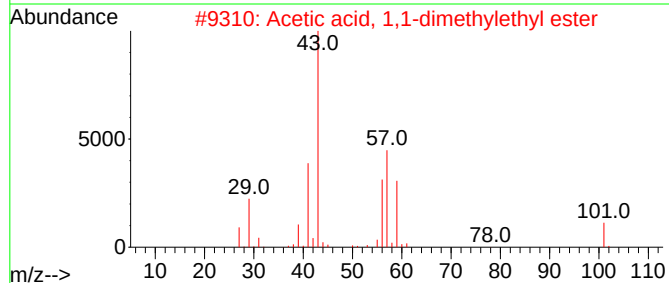
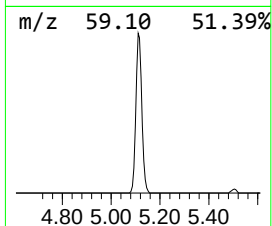
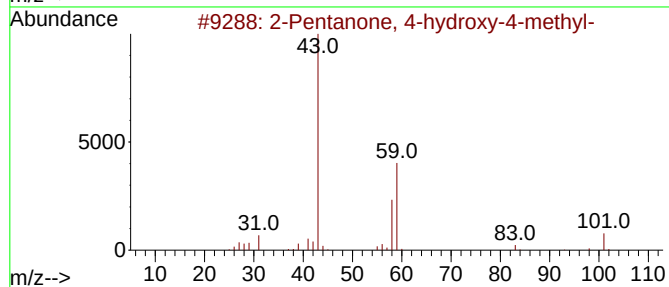
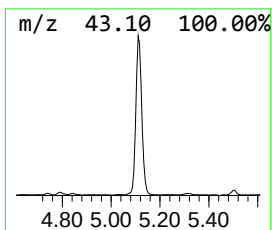
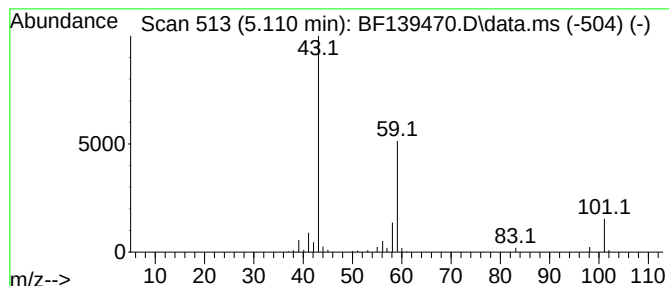
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	7.44 ng	193585	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	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		



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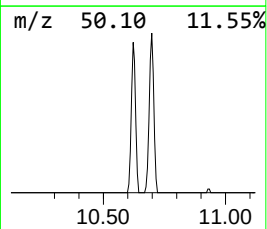
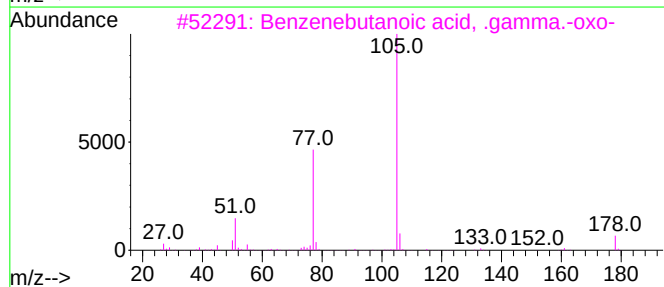
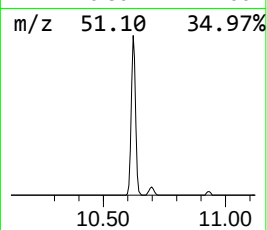
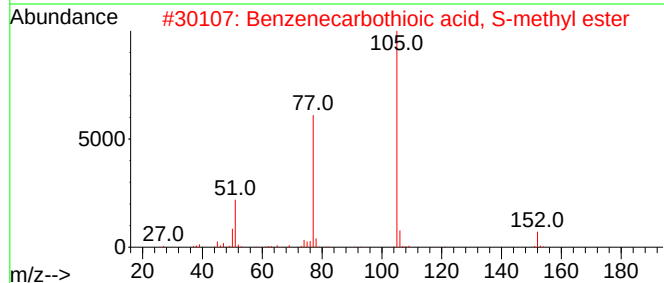
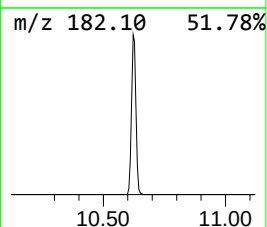
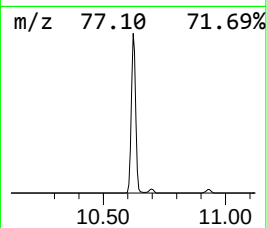
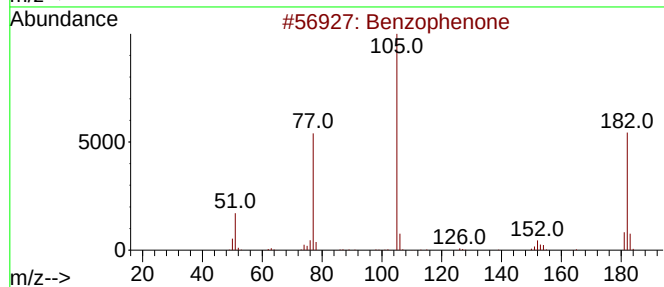
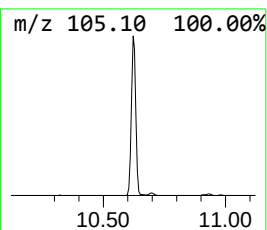
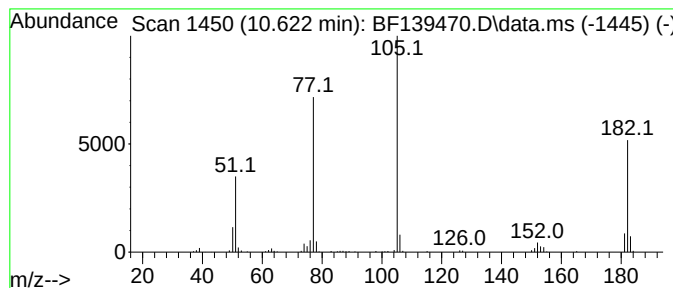
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	6.61 ng	229370	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	64
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50



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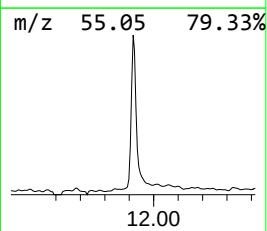
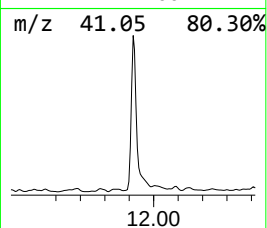
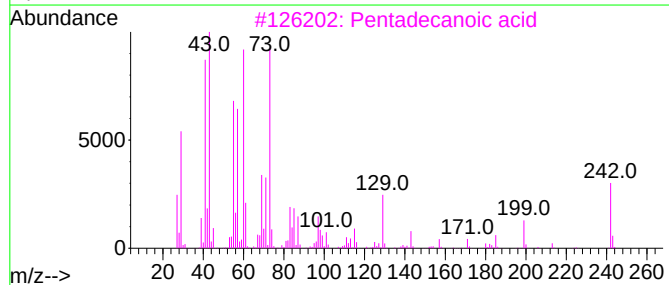
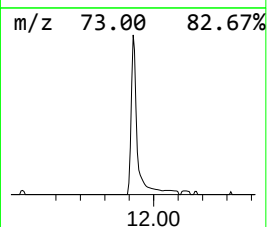
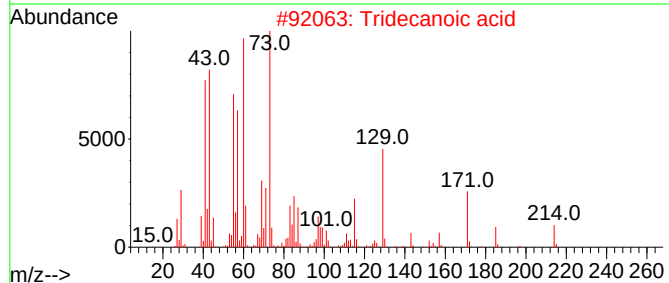
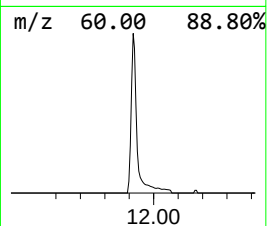
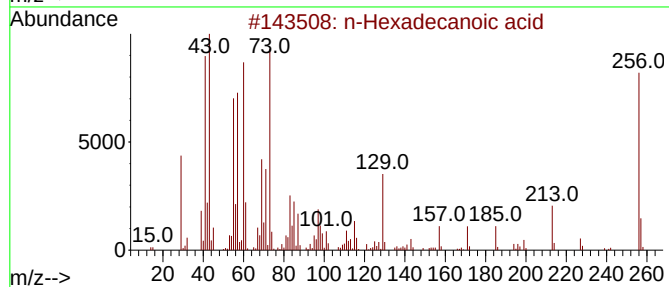
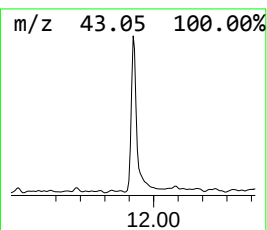
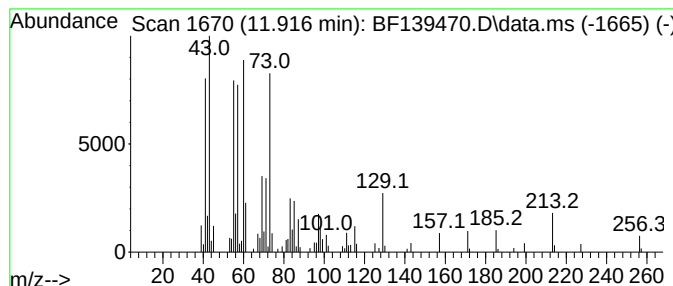
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	4.76 ng	146377	Phenanthrene-d10	11.398

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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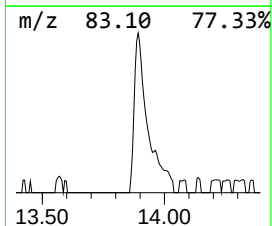
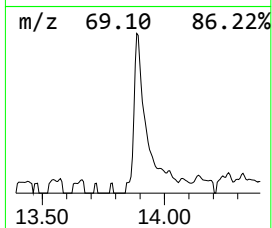
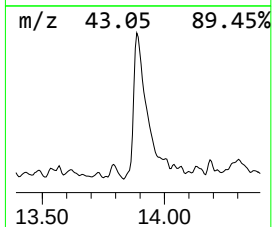
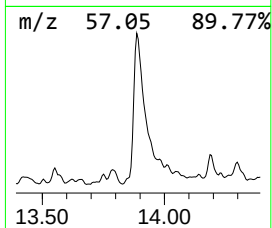
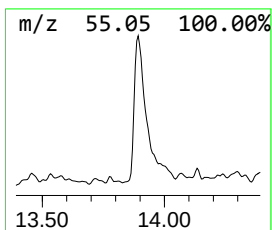
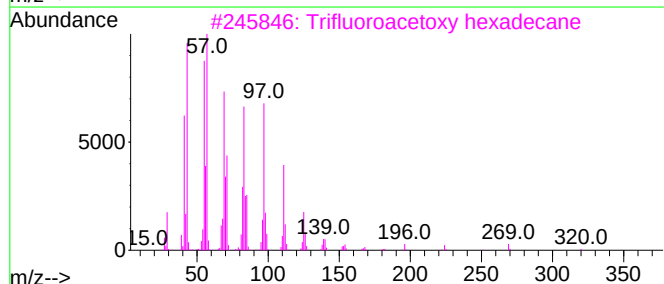
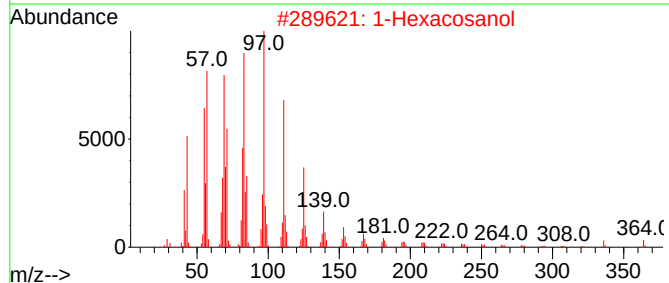
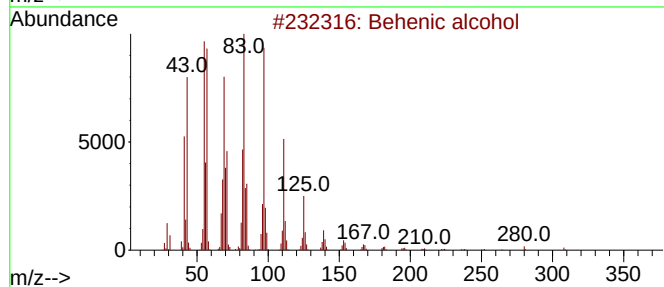
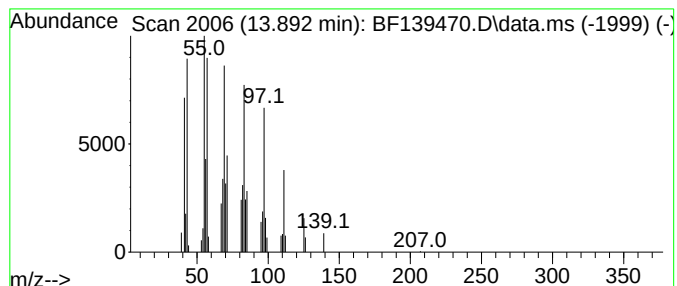
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	5.87 ng	98578	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	91
2			1-Hexacosanol	382	C26H54O	000506-52-5	91
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			1-Hexacosene	364	C26H52	018835-33-1	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...	2.222	76.7	ng	1993910	1	6.875	520206	20.0
2-Pentanone, 4-...	5.110	7.4	ng	193585	1	6.875	520206	20.0
Benzophenone	10.622	6.6	ng	229370	3	9.910	693850	20.0
n-Hexadecanoic ...	11.916	4.8	ng	146377	4	11.398	614654	20.0
Behenic alcohol	13.892	5.9	ng	98578	5	14.027	335758	20.0