

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091924\
 Data File : BF139463.D
 Acq On : 19 Sep 2024 14:37
 Operator : RC/JU
 Sample : P4087-19
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-614-COMP-04

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: BF139463.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	11	19	29	rVB	715951	1110299	62.34%	8.390%
2	5.099	501	511	519	rBV	88793	133984	7.52%	1.012%
3	5.499	573	579	584	rBV	1213027	1583729	88.92%	11.968%
4	6.504	744	750	755	rBV	1248342	1693346	95.07%	12.796%
5	6.875	808	813	818	rBV	384715	481524	27.04%	3.639%
6	7.440	903	909	914	rBV	822558	1062793	59.67%	8.031%
7	7.693	947	952	957	rVB	24541	31113	1.75%	0.235%
8	8.157	1026	1031	1036	rBV	487852	595550	33.44%	4.500%
9	8.375	1061	1068	1074	rBV2	16925	21229	1.19%	0.160%
10	9.234	1208	1214	1219	rBV	1427617	1781095	100.00%	13.459%
11	9.910	1324	1329	1334	rBV	512072	626961	35.20%	4.738%
12	10.622	1445	1450	1457	rVB	65703	79604	4.47%	0.602%
13	10.698	1457	1463	1479	rBV	830186	1048658	58.88%	7.924%
14	11.398	1576	1582	1589	rBV	461972	599115	33.64%	4.527%
15	11.916	1665	1670	1686	rBV	115305	185472	10.41%	1.402%
16	12.704	1799	1804	1812	rBV	13266	22350	1.25%	0.169%
17	12.980	1845	1851	1856	rBV	1072232	1353080	75.97%	10.225%
18	13.545	1942	1947	1955	rVB2	12400	18896	1.06%	0.143%
19	13.880	1999	2004	2024	rBV2	44393	131312	7.37%	0.992%
20	14.027	2024	2029	2035	rBV	252672	327501	18.39%	2.475%
21	15.145	2214	2219	2228	rVB	12698	19399	1.09%	0.147%
22	15.498	2273	2279	2290	rBV	199245	326197	18.31%	2.465%

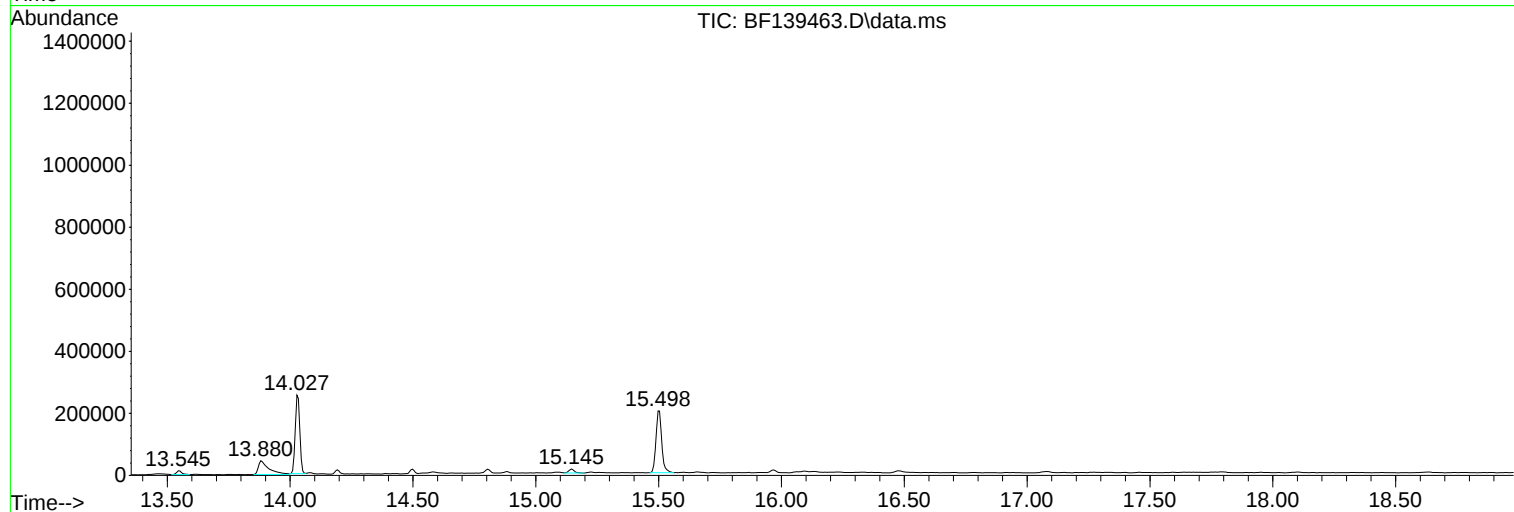
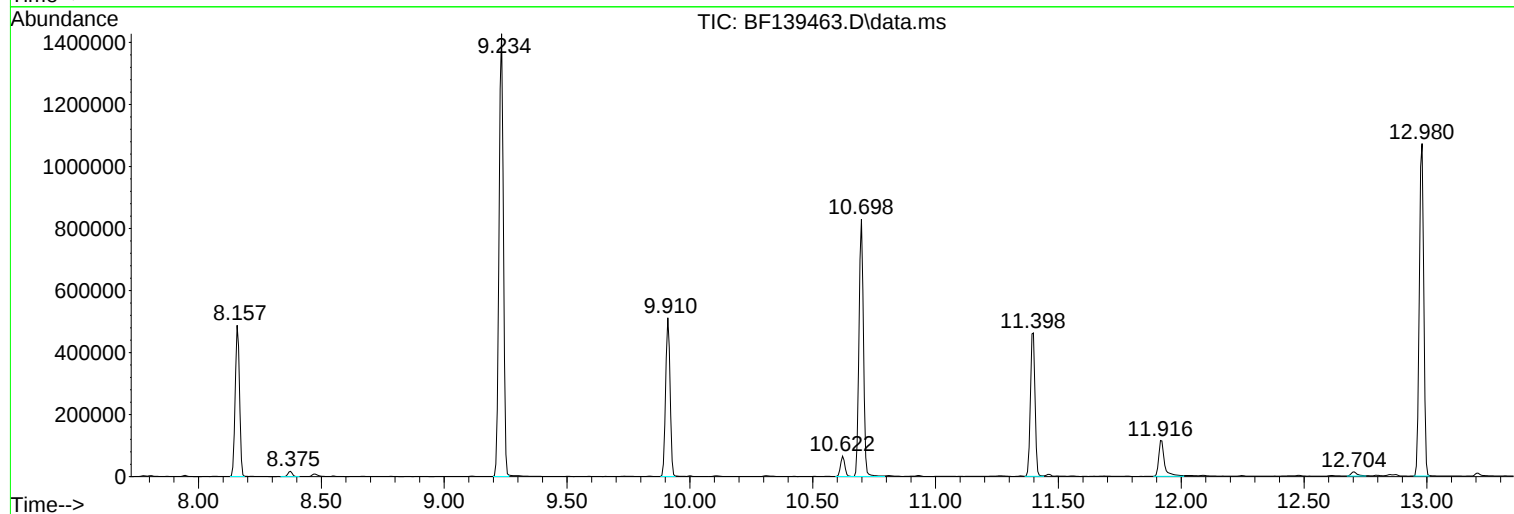
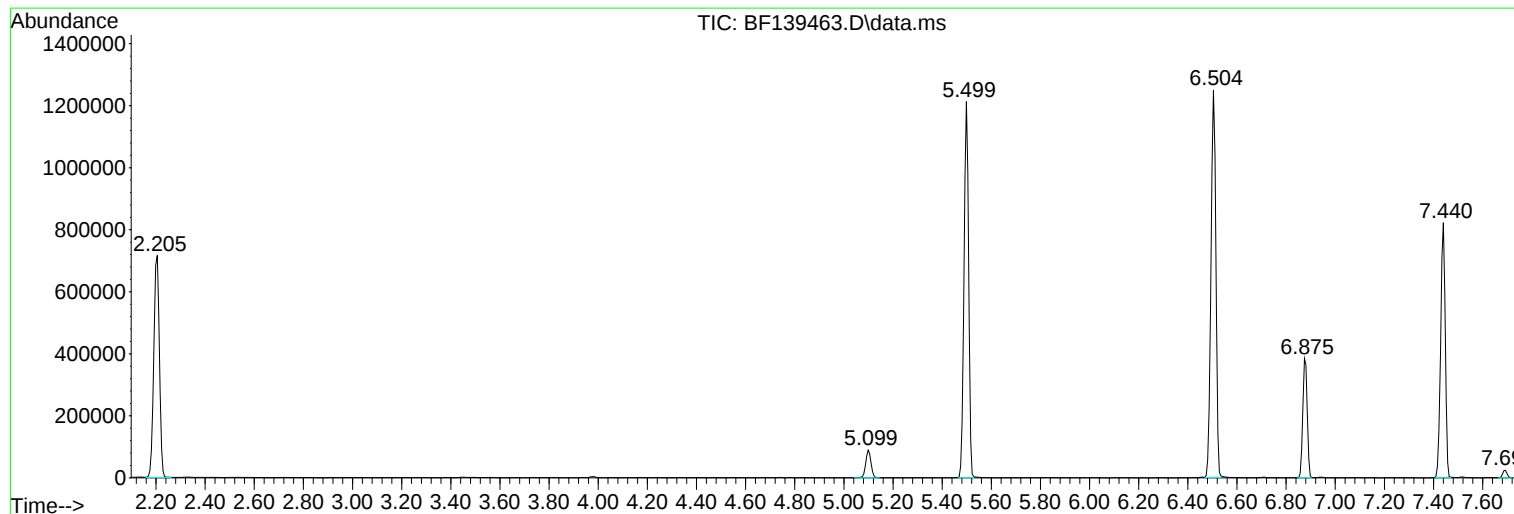
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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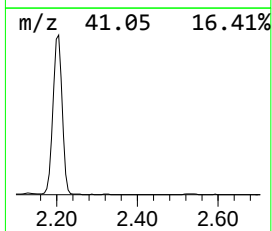
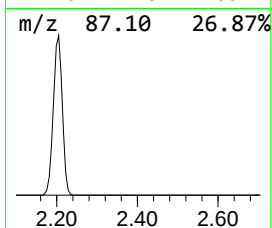
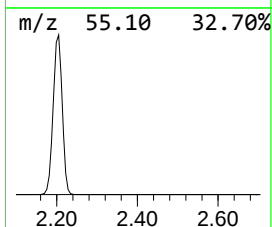
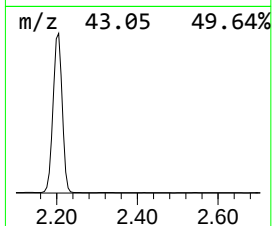
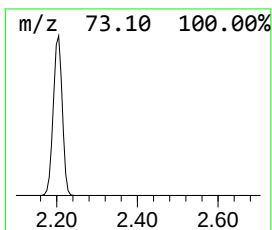
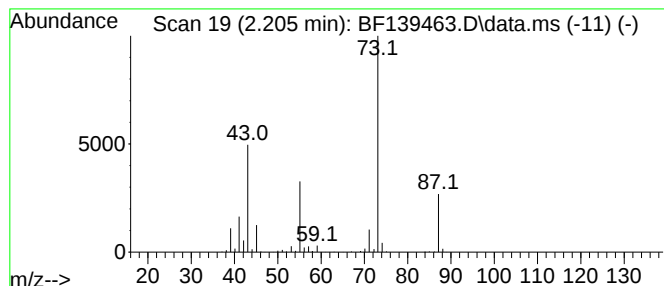
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.205	46.12 ng	1110300	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			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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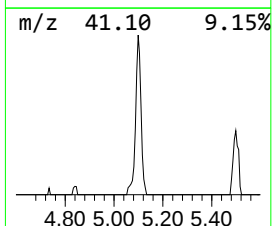
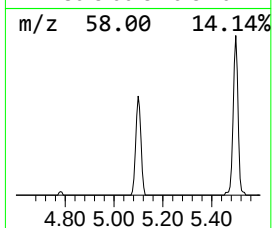
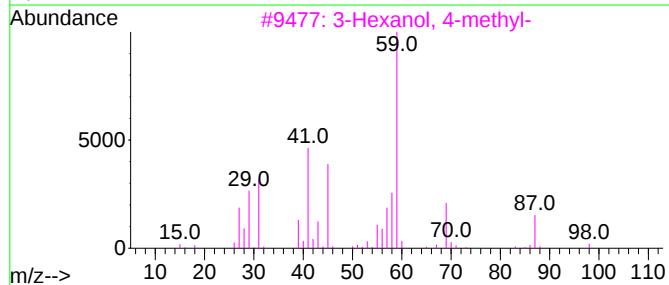
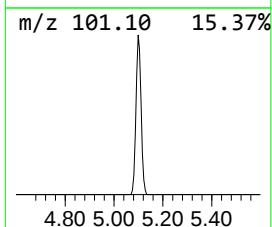
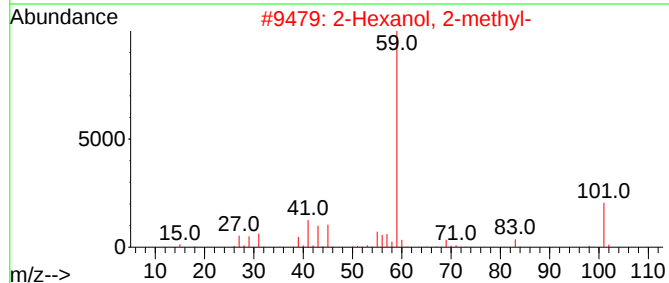
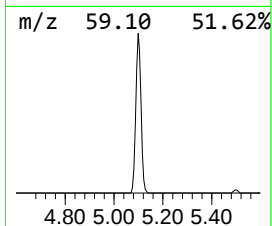
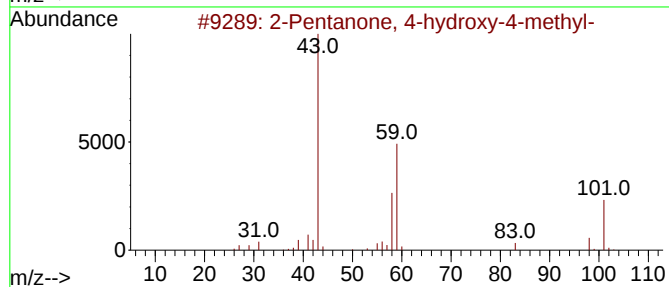
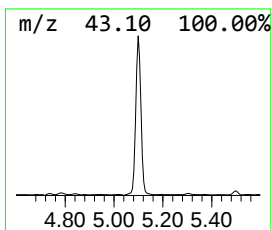
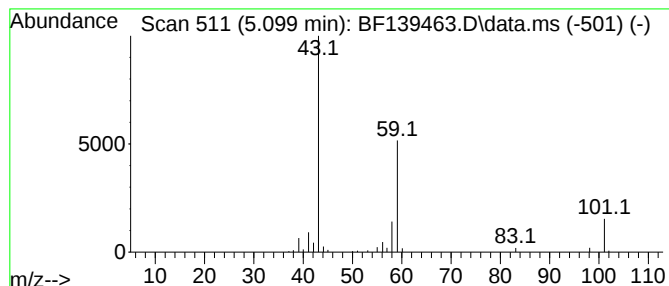
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	5.57 ng	133984	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		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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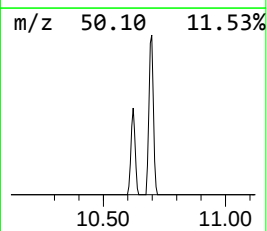
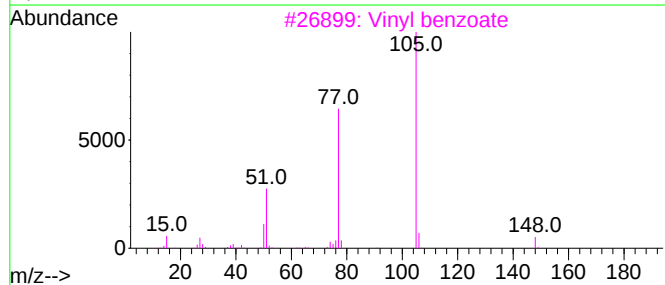
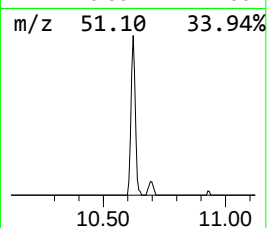
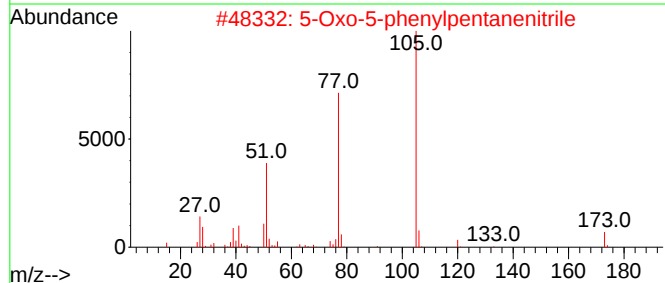
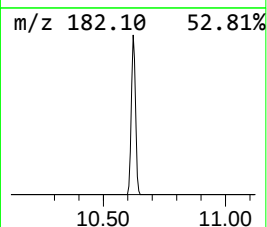
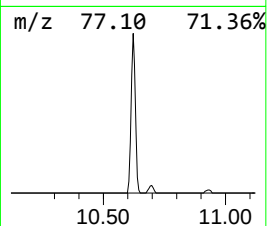
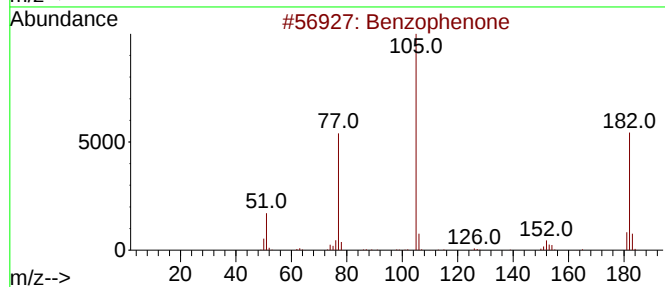
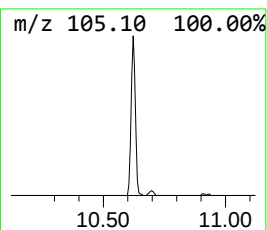
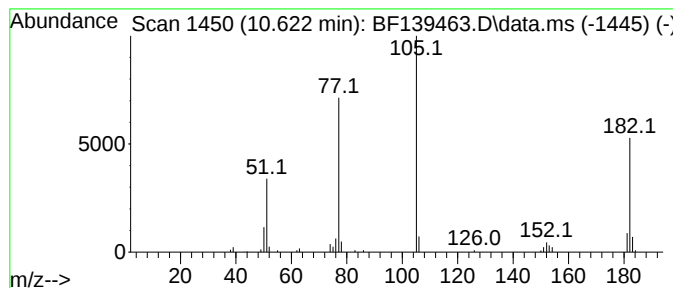
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	2.54 ng	79604	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	50
3			Vinyl benzoate	148	C9H8O2	000769-78-8	50
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
5			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	50



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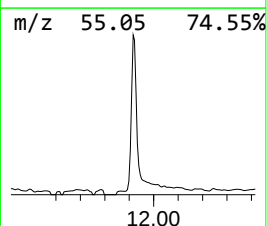
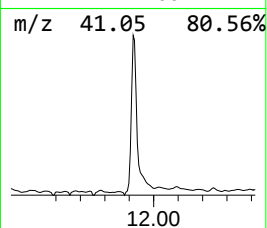
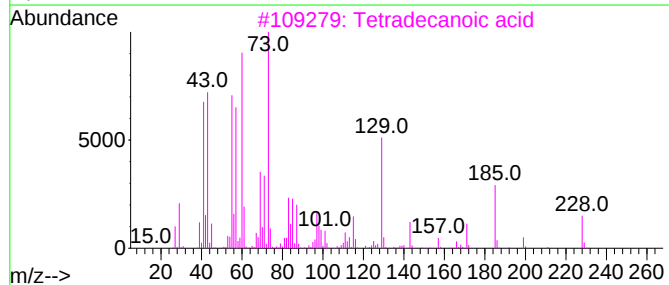
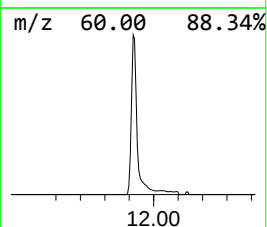
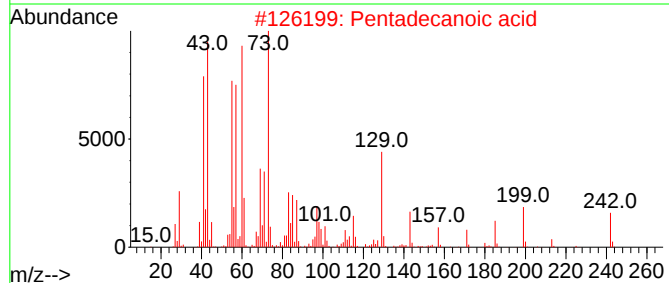
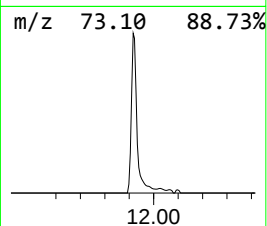
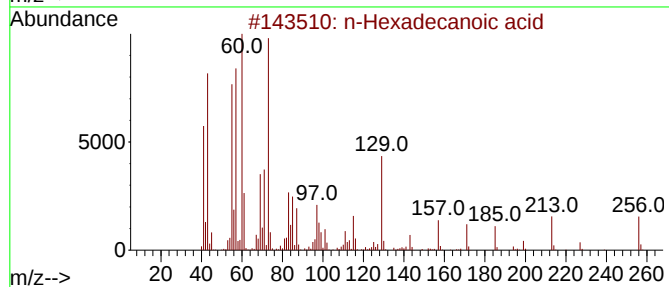
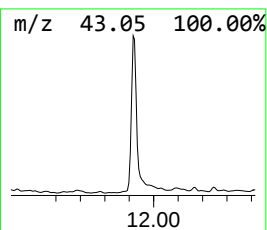
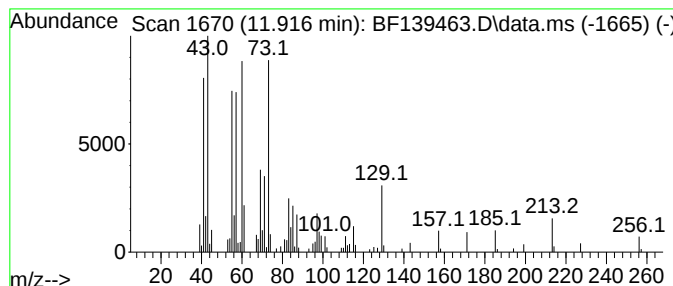
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	6.19 ng	185472	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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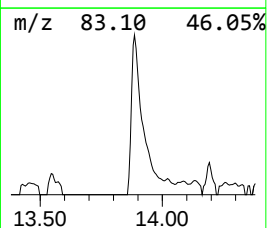
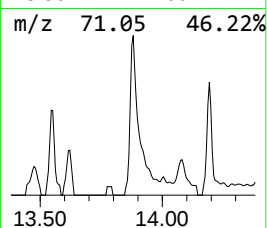
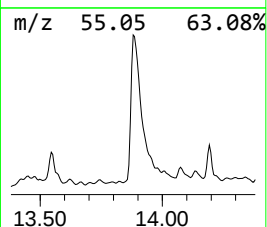
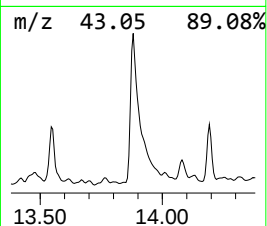
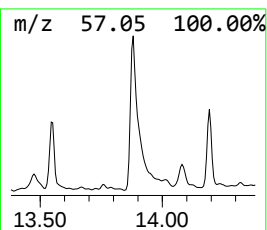
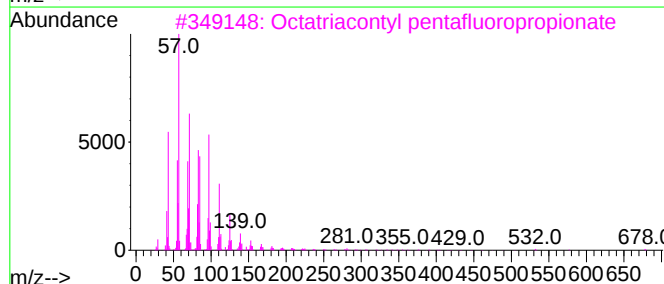
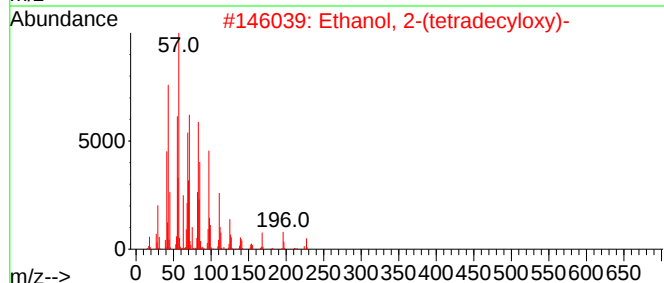
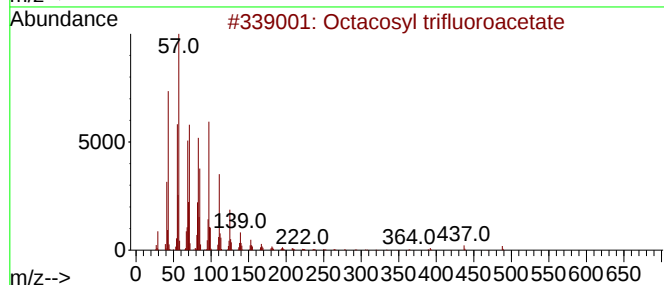
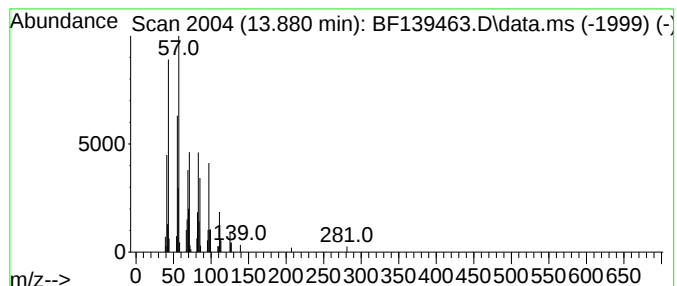
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	8.02 ng	131312	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	91
4			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	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...	2.205	46.1	ng	1110300	1	6.875	481524	20.0
2-Pentanone, 4-...	5.099	5.6	ng	133984	1	6.875	481524	20.0
Benzophenone	10.622	2.5	ng	79604	3	9.910	626961	20.0
n-Hexadecanoic ...	11.916	6.2	ng	185472	4	11.398	599115	20.0
Octacosyl trifl...	13.880	8.0	ng	131312	5	14.027	327501	20.0