

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
 Data File : BF139859.D
 Acq On : 18 Oct 2024 17:44
 Operator : RC/JU
 Sample : P4425-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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: BF139859.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	14	22	rVB	1782732	2875269	100.00%	12.861%
2	5.110	505	513	521	rVB	142433	217735	7.57%	0.974%
3	5.498	573	579	585	rBV	2037959	2731665	95.01%	12.219%
4	6.504	743	750	755	rBV	1942095	2628119	91.40%	11.755%
5	6.886	810	815	821	rBV	685593	874281	30.41%	3.911%
6	7.445	904	910	915	rBV	1252721	1548533	53.86%	6.927%
7	7.698	948	953	958	rBV	78250	92711	3.22%	0.415%
8	8.169	1028	1033	1038	rBV	818853	993017	34.54%	4.442%
9	9.245	1210	1216	1221	rBV	1918983	2335947	81.24%	10.449%
10	9.922	1326	1331	1337	rVB	703391	892990	31.06%	3.994%
11	10.633	1447	1452	1458	rBV	328809	410860	14.29%	1.838%
12	10.710	1460	1465	1478	rVB	1008574	1253784	43.61%	5.608%
13	11.410	1579	1584	1591	rBV	756378	928993	32.31%	4.155%
14	11.933	1665	1673	1685	rBV	147965	252240	8.77%	1.128%
15	12.621	1786	1790	1801	rBV	32306	52237	1.82%	0.234%
16	12.721	1802	1807	1814	rBV3	32213	55595	1.93%	0.249%
17	12.851	1825	1829	1835	rVB	25862	33279	1.16%	0.149%
18	12.998	1848	1854	1859	rBV	1924026	2462400	85.64%	11.014%
19	13.892	2002	2006	2017	rBV	139497	244072	8.49%	1.092%
20	14.045	2027	2032	2045	rBV	660114	916697	31.88%	4.100%
21	15.527	2278	2284	2289	rBV	366814	556082	19.34%	2.487%

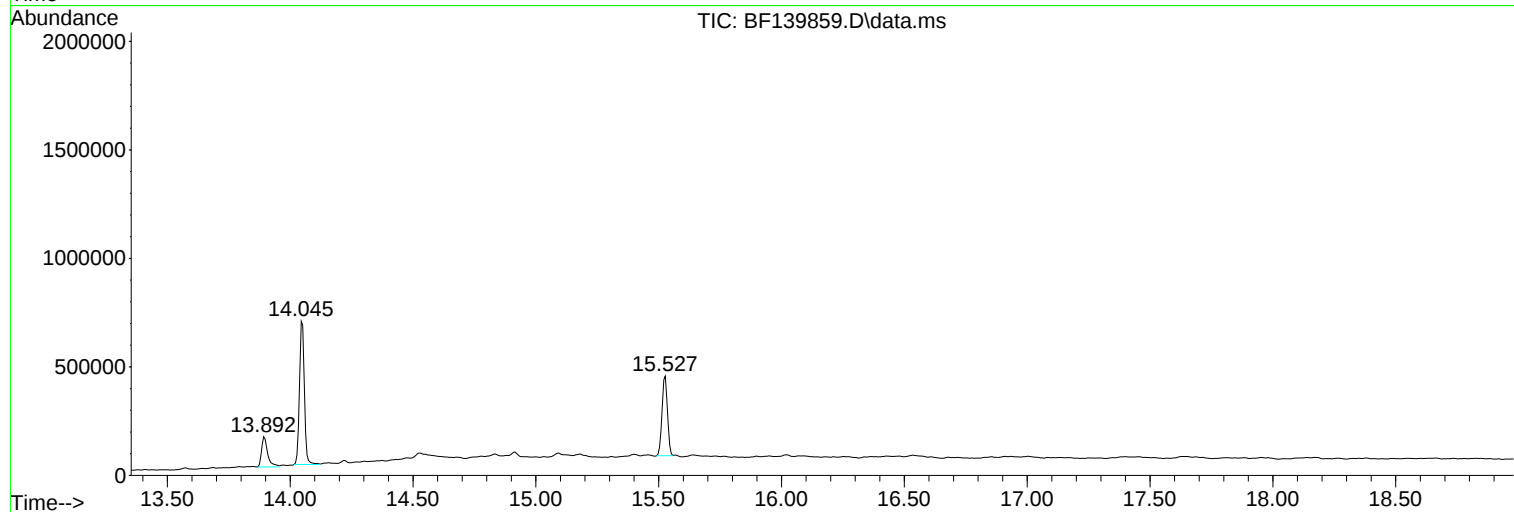
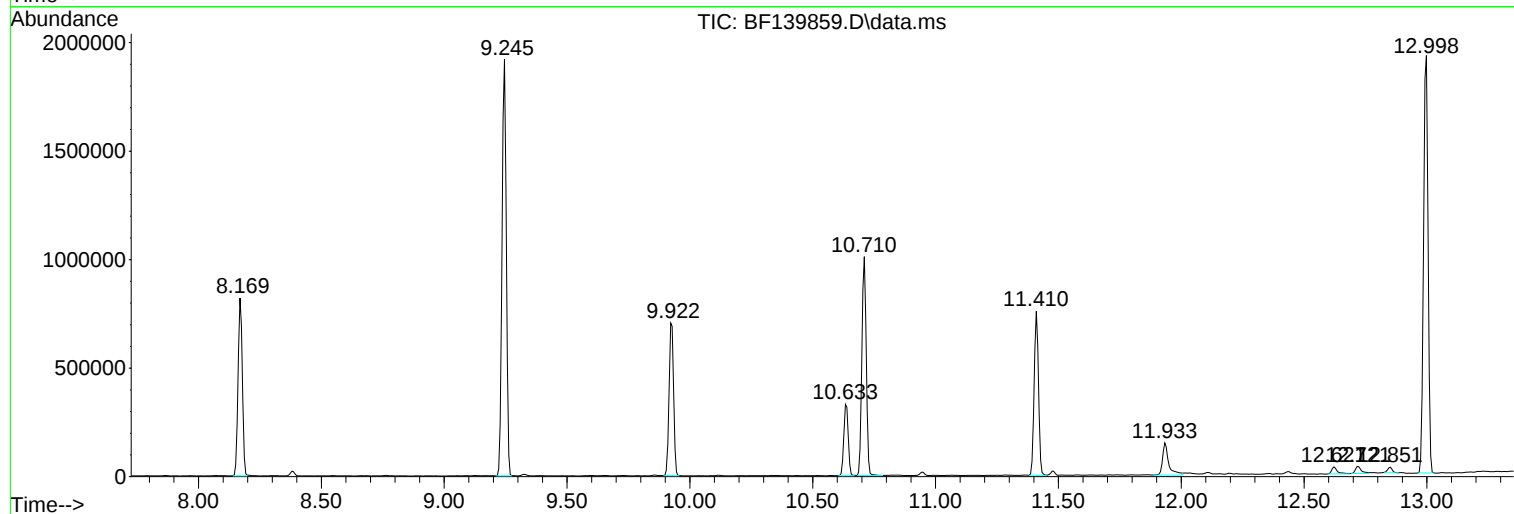
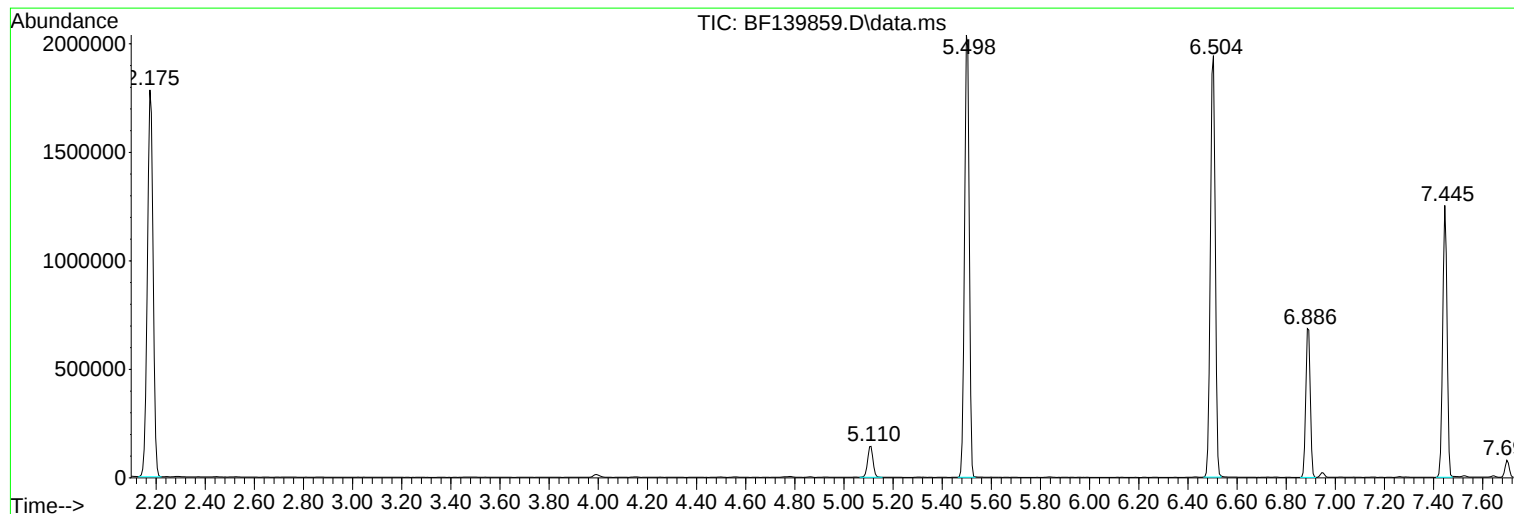
Sum of corrected areas: 22356506

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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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139859.D
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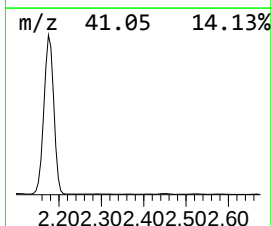
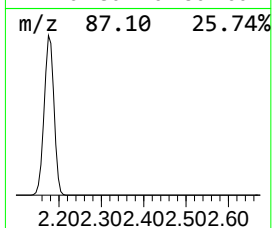
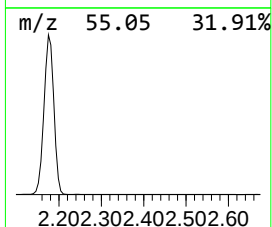
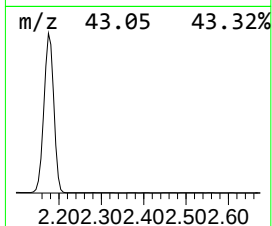
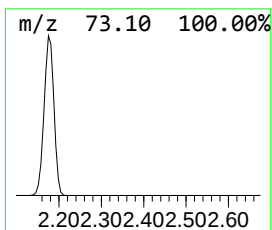
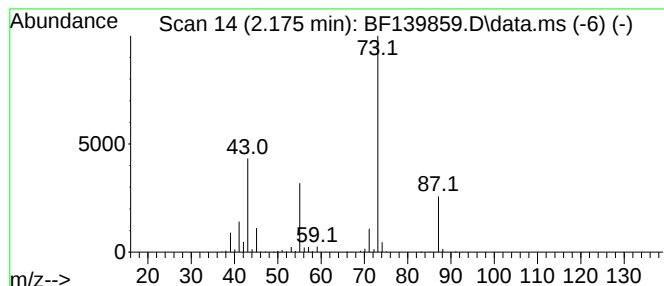
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	65.77 ng	2875270	1,4-Dichlorobenzene-d4	6.892

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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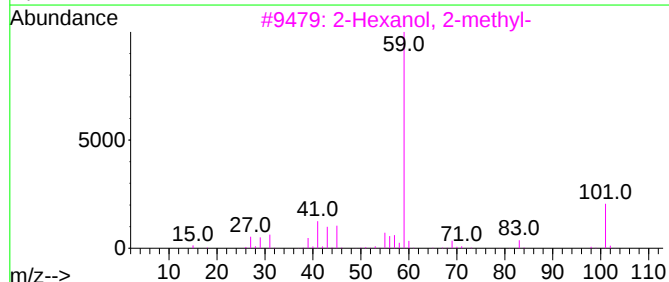
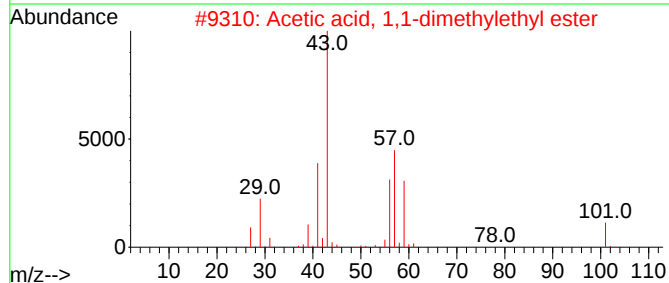
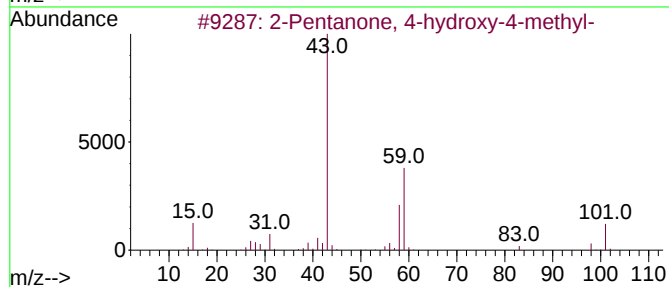
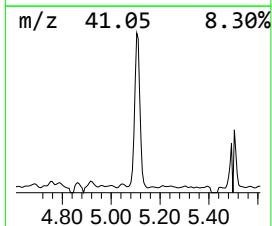
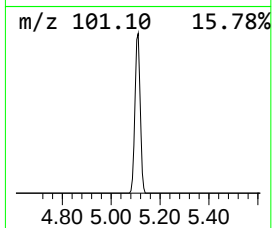
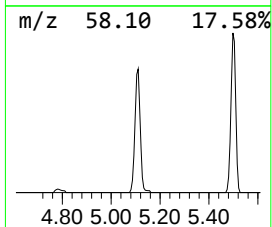
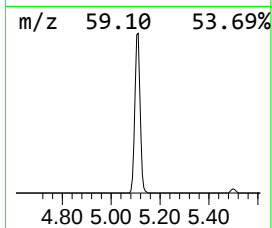
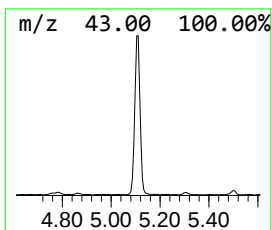
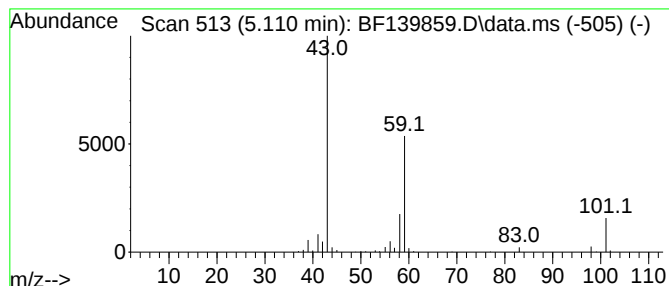
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	4.98 ng	217735	1,4-Dichlorobenzene-d4	6.892

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		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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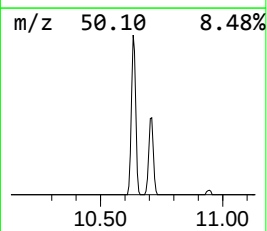
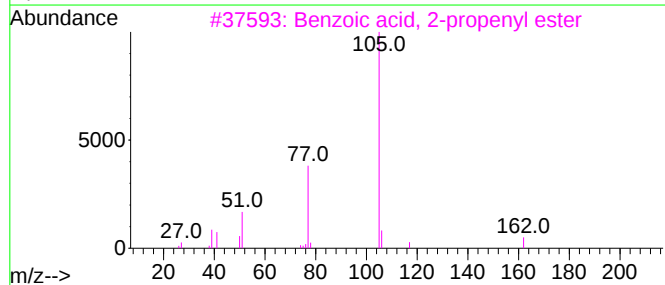
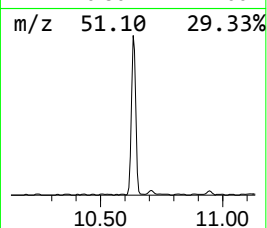
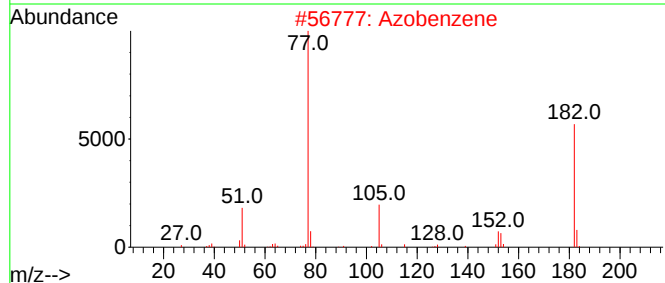
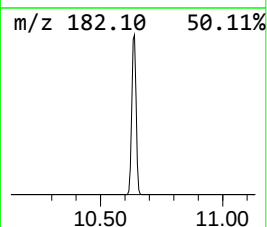
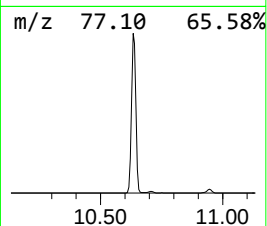
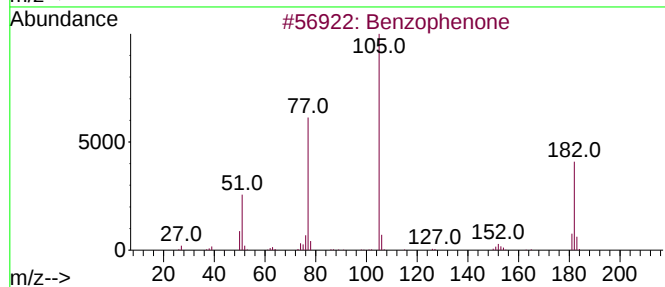
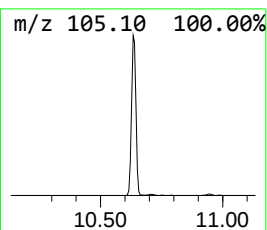
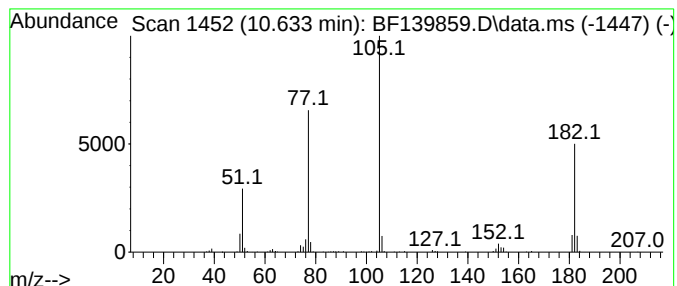
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	9.20 ng	410860	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	47
4			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
5			N-Methylbenzamide, N-heptafluoro...	331	C12H8F7NO2	1000446-97-2	47



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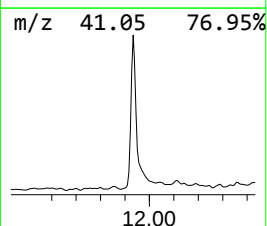
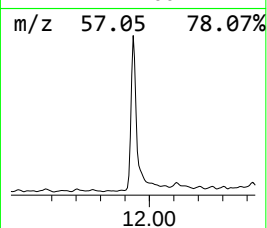
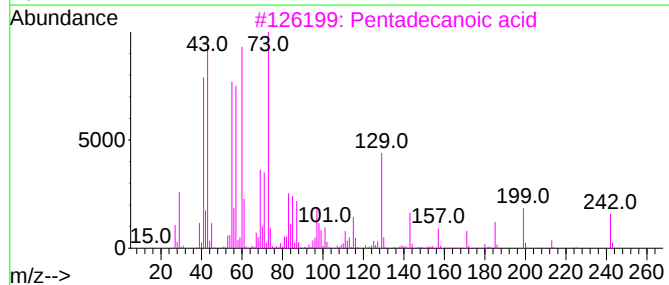
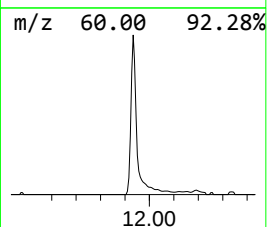
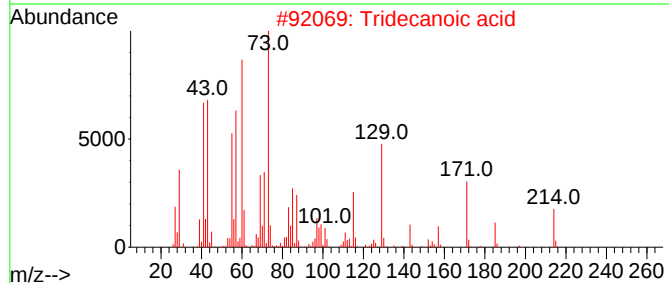
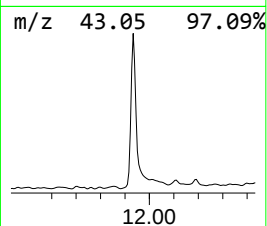
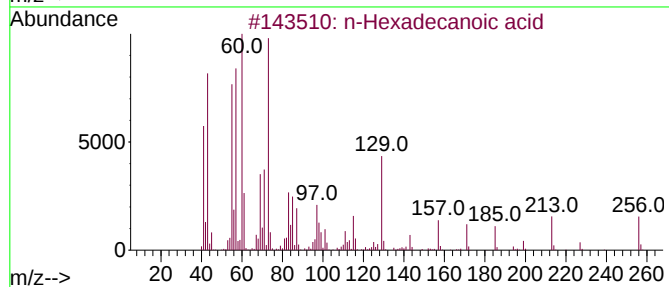
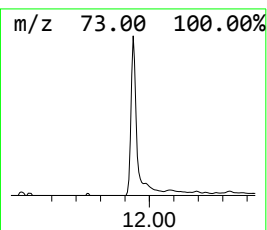
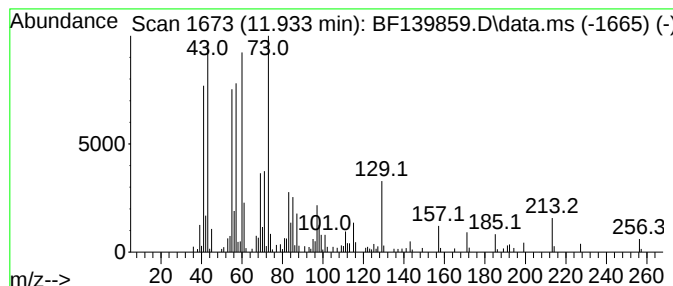
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	5.43 ng	252240	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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	50



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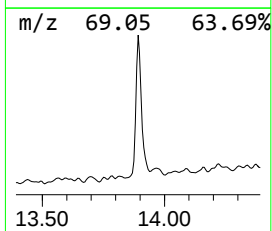
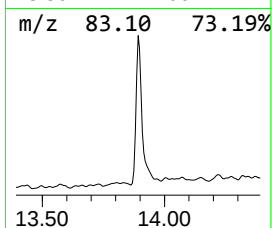
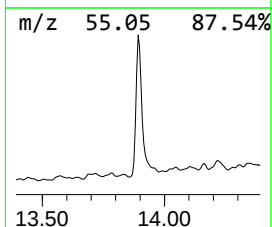
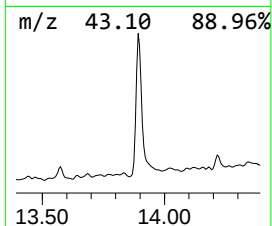
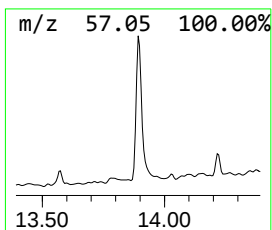
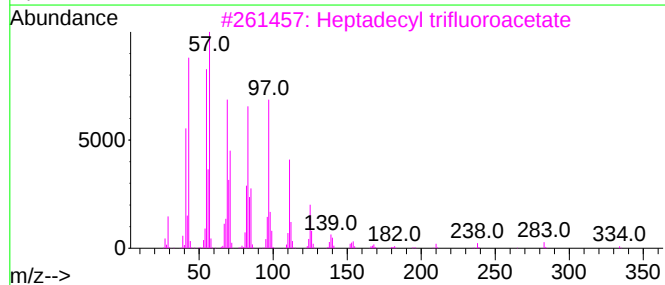
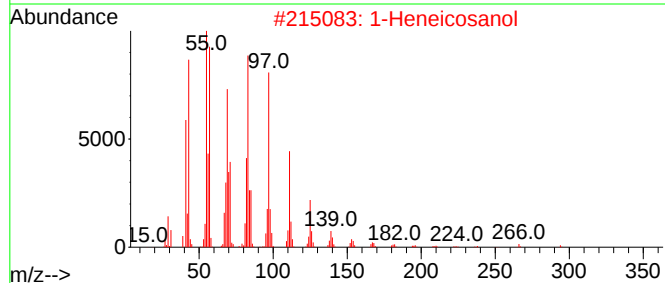
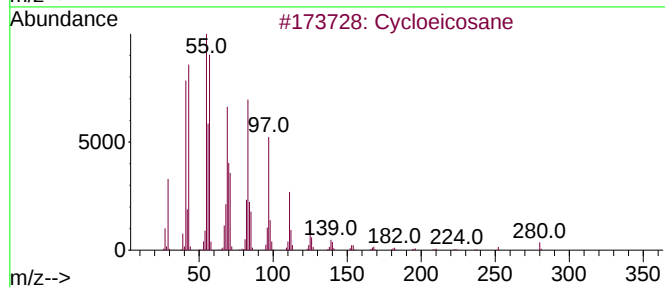
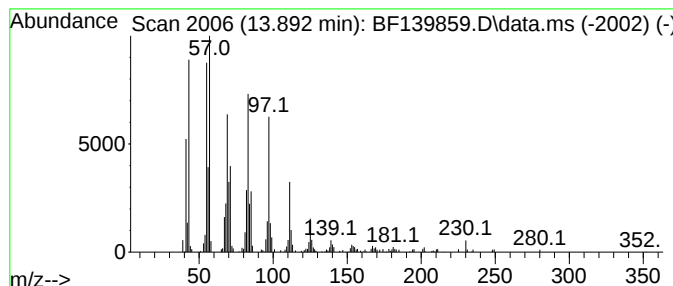
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Cycloeicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	5.33 ng	244072	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	98
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
4			1-Docosene	308	C22H44	001599-67-3	94
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	65.8	ng	2875270	1	6.892	874281	20.0
2-Pentanone, 4-...	5.110	5.0	ng	217735	1	6.892	874281	20.0
Benzophenone	10.633	9.2	ng	410860	3	9.922	892990	20.0
n-Hexadecanoic ...	11.933	5.4	ng	252240	4	11.410	928993	20.0
Cycloeicosane	13.892	5.3	ng	244072	5	14.045	916697	20.0