

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053023\
 Data File : BF133526.D
 Acq On : 30 May 2023 17:19
 Operator : CG\JU
 Sample : 02955-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB21

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133526.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	3	11	16	rVB	209533	285854	6.51%	0.982%
2	5.063	498	506	515	rVB	166900	218960	4.99%	0.752%
3	5.451	566	572	575	rBV	3513128	3756244	85.59%	12.901%
4	6.457	737	743	746	rBV	3226300	3893800	88.72%	13.373%
5	6.828	803	806	810	rBV	988908	859026	19.57%	2.950%
6	7.398	897	903	906	rBV	2604465	2463779	56.14%	8.462%
7	8.116	1021	1025	1028	rVB	1337321	1114448	25.39%	3.828%
8	9.192	1202	1208	1211	rBV	4509933	4177197	95.18%	14.347%
9	9.869	1319	1323	1326	rBV	1525542	1190802	27.13%	4.090%
10	10.586	1441	1445	1448	rBV	212443	162937	3.71%	0.560%
11	10.657	1453	1457	1461	rBV	2770892	2771664	63.15%	9.519%
12	11.357	1572	1576	1579	rBV	1519498	1278887	29.14%	4.392%
13	11.886	1662	1666	1670	rBV	236958	211216	4.81%	0.725%
14	12.951	1842	1847	1850	rBV	4431384	4388718	100.00%	15.073%
15	13.857	1996	2001	2016	rBV	178196	307359	7.00%	1.056%
16	13.998	2020	2025	2029	rBV	1266769	1107283	25.23%	3.803%
17	14.480	2103	2107	2112	rBV	38545	49439	1.13%	0.170%
18	15.127	2212	2217	2221	rBV2	37387	45861	1.04%	0.158%
19	15.456	2267	2273	2278	rBV	657535	787644	17.95%	2.705%
20	15.939	2351	2355	2360	rBV	32197	45295	1.03%	0.156%

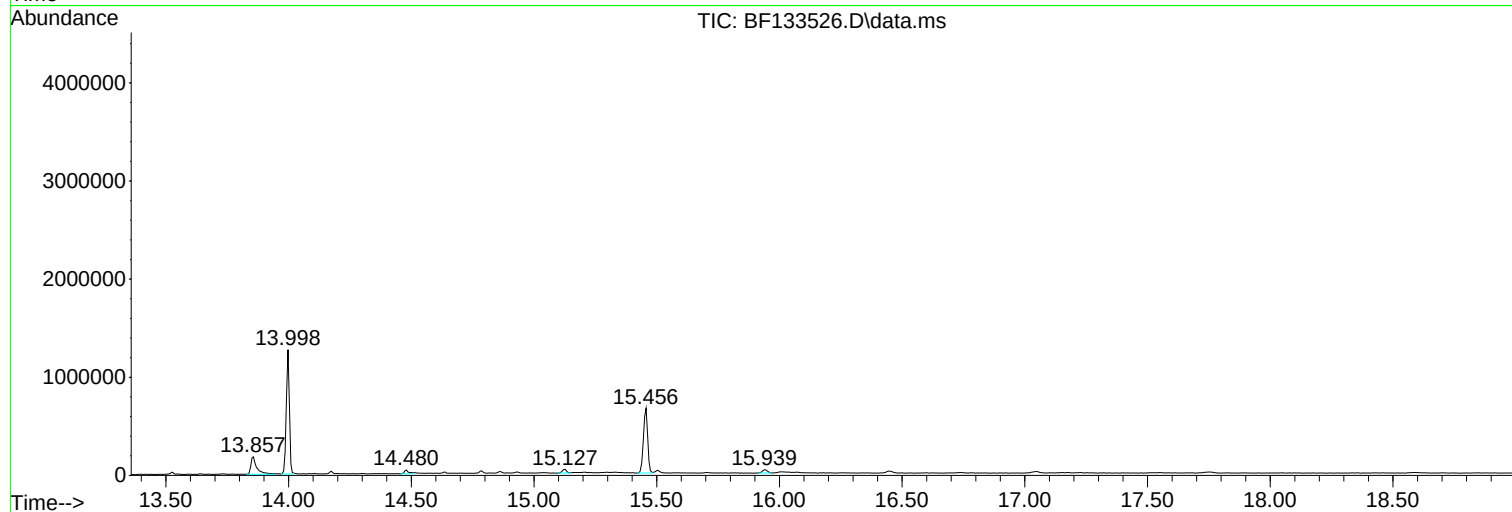
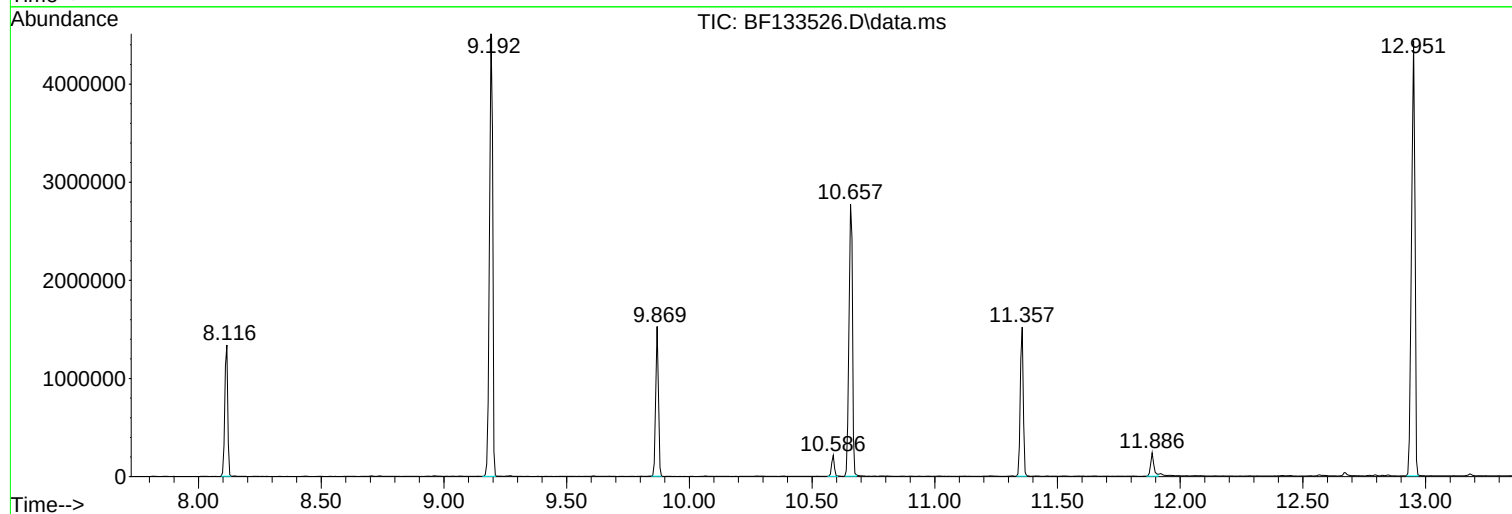
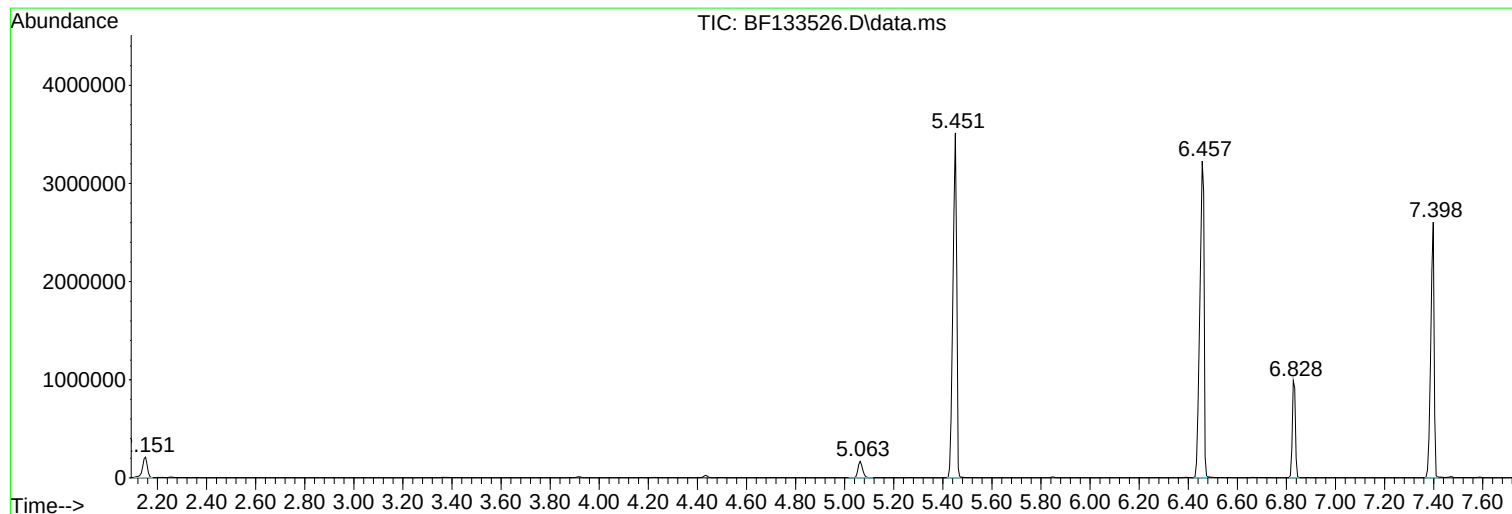
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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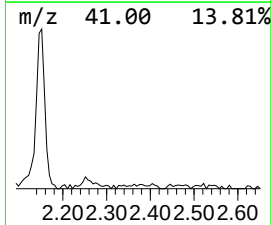
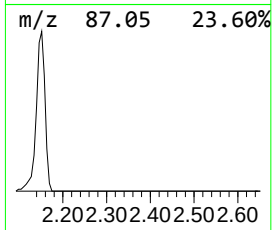
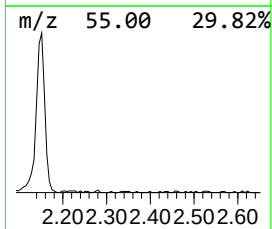
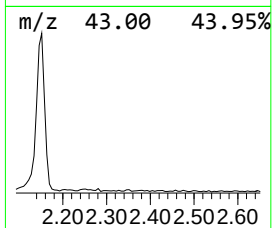
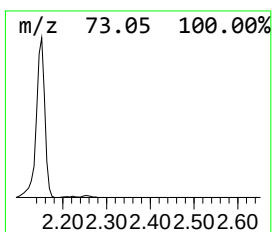
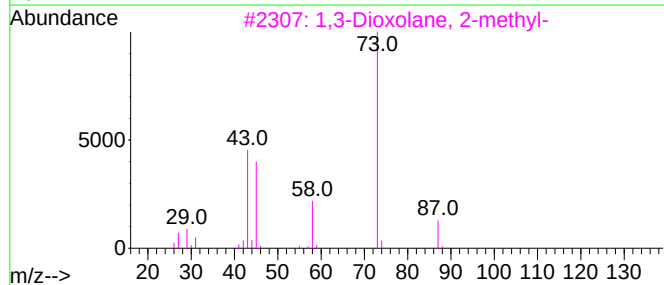
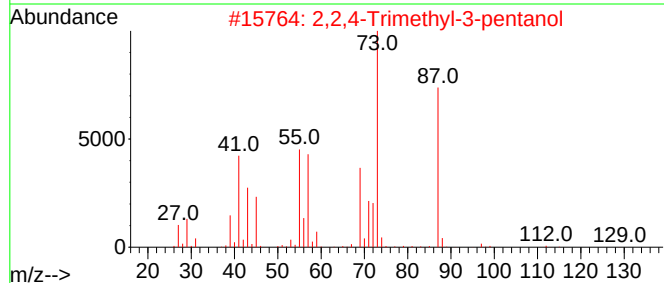
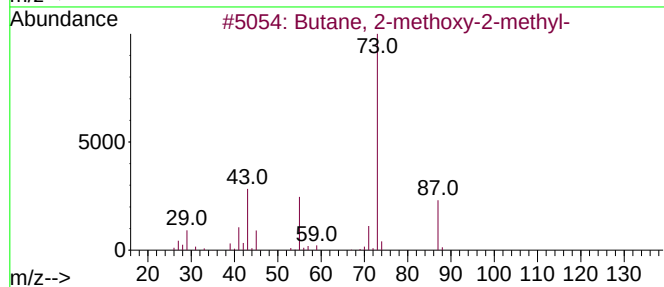
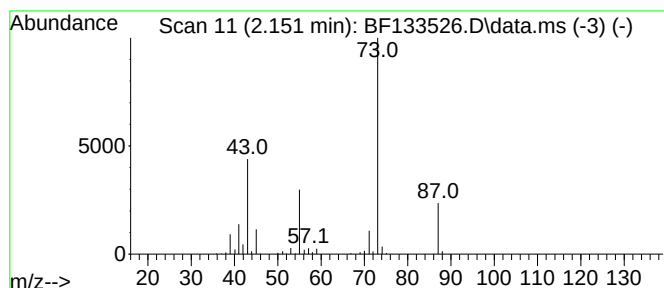
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.151	6.66 ng	285854	1,4-Dichlorobenzene-d4	6.833

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	38
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17



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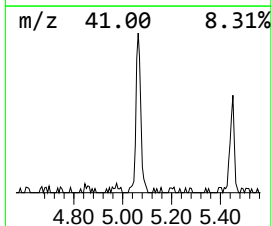
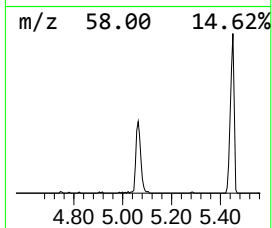
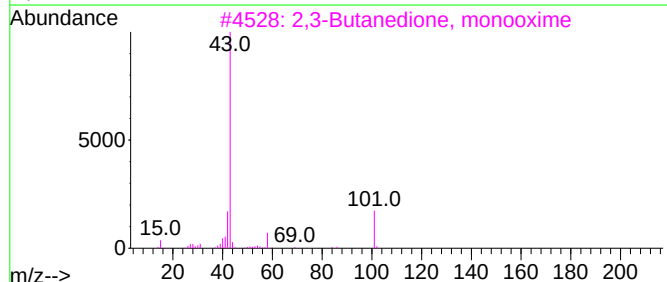
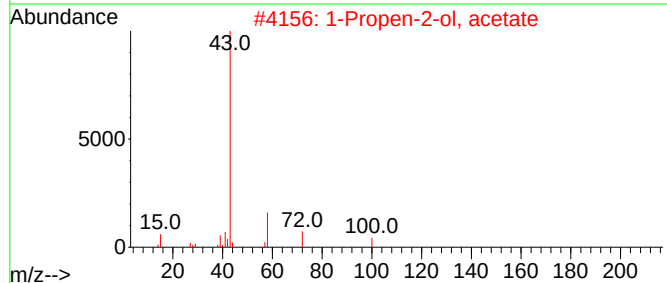
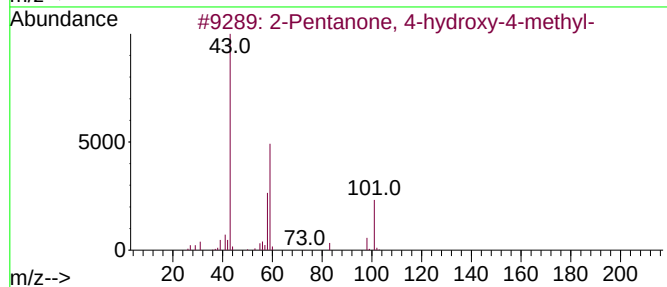
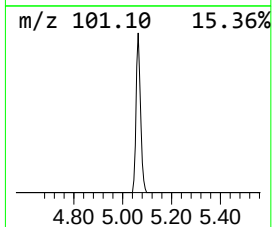
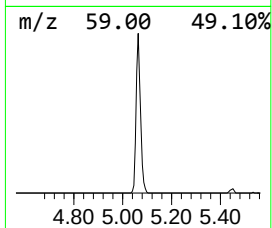
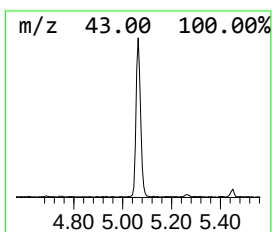
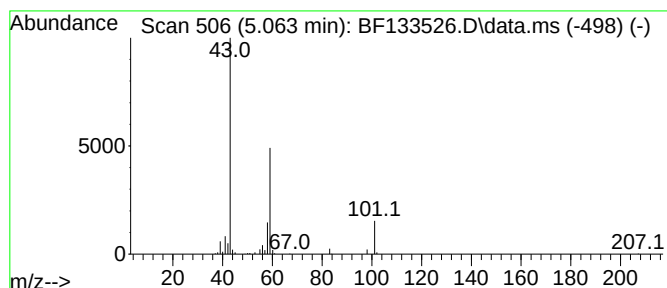
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	5.10 ng	218960	1,4-Dichlorobenzene-d4	6.833

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	7



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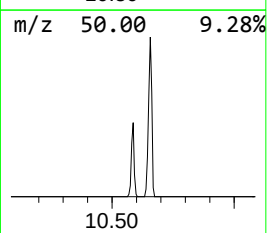
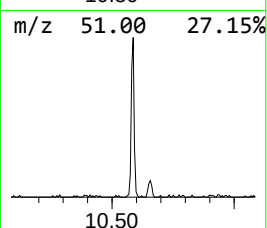
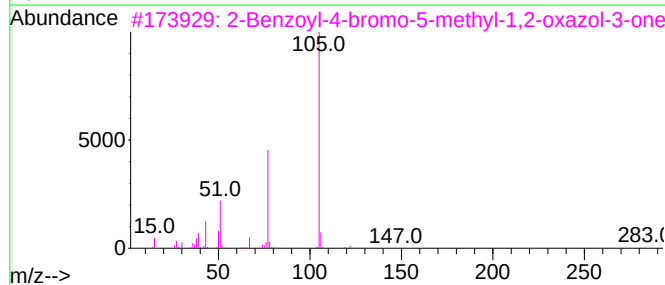
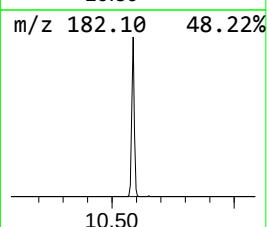
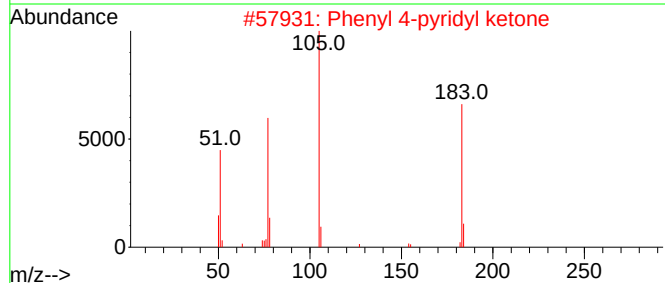
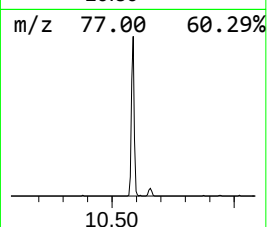
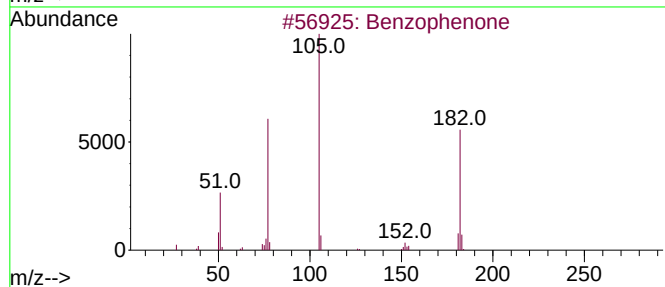
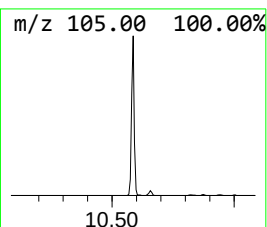
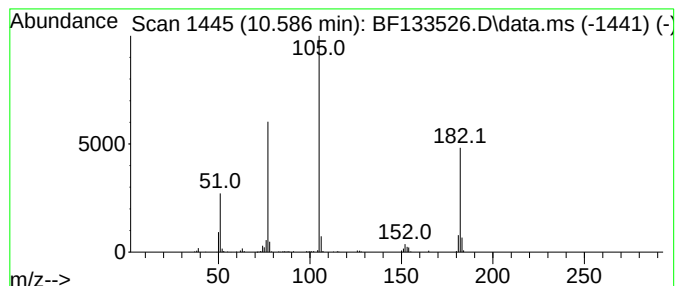
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	2.74 ng	162937	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	52
3			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	50
5			Vinyl benzoate	148	C9H8O2	000769-78-8	50



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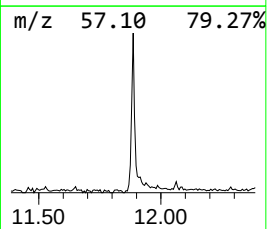
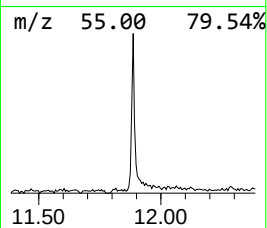
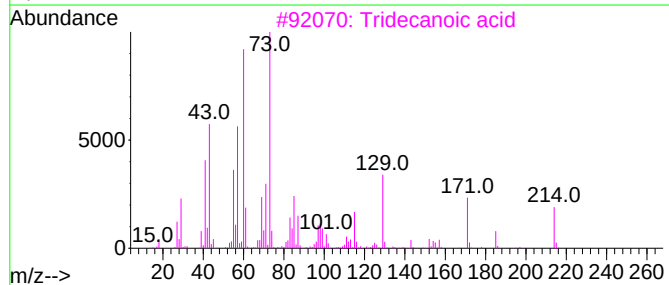
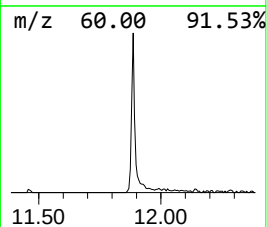
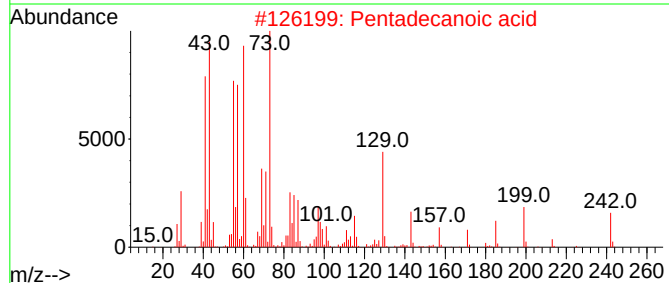
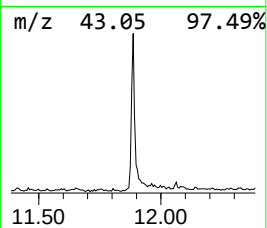
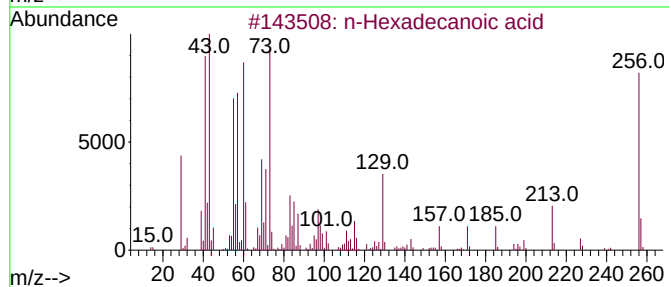
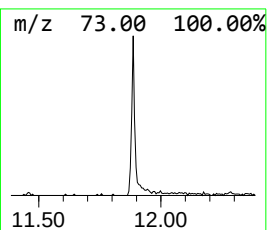
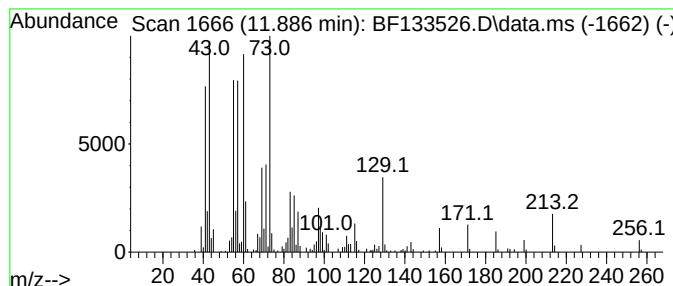
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.30 ng	211216	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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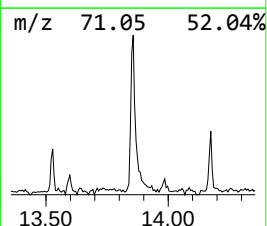
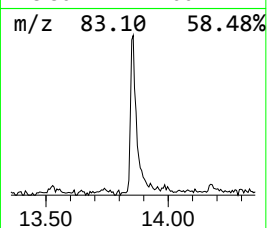
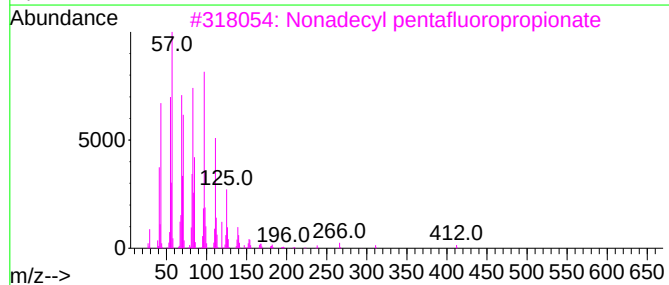
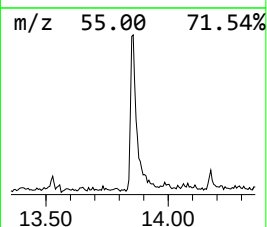
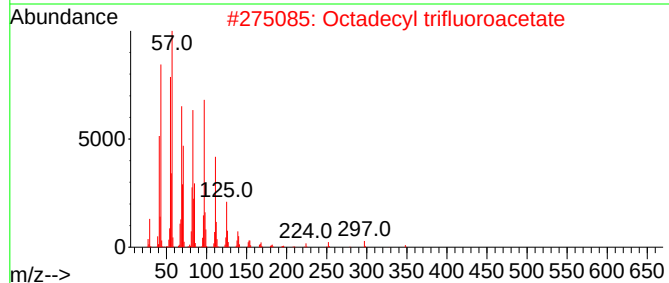
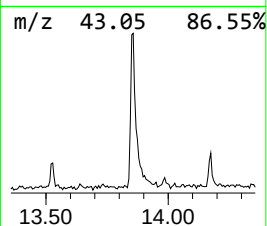
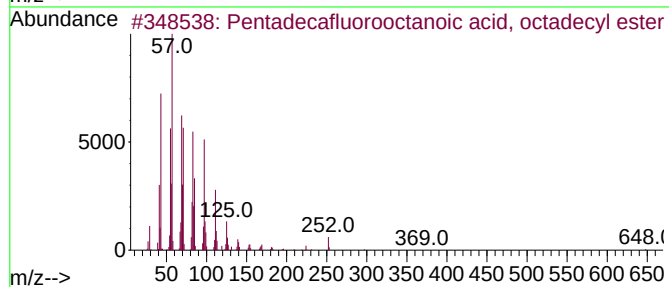
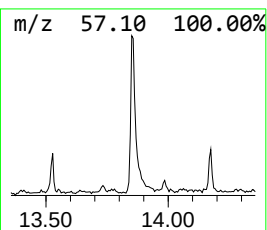
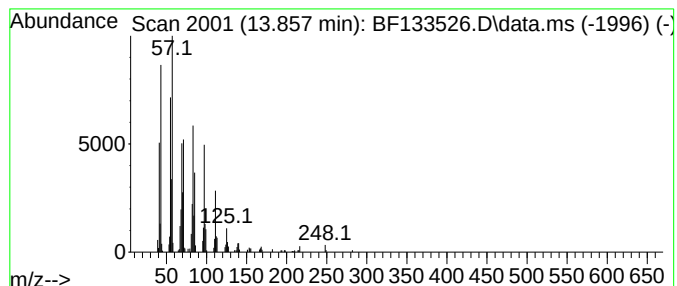
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.857	5.55 ng	307359	Chrysene-d12	13.998	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	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...	2.151	6.7	ng	285854	1	6.833	859026	20.0
2-Pentanone, 4-...	5.063	5.1	ng	218960	1	6.833	859026	20.0
Benzophenone	10.586	2.7	ng	162937	3	9.869	1190800	20.0
n-Hexadecanoic ...	11.886	3.3	ng	211216	4	11.357	1278890	20.0
Pentadecafluoro...	13.857	5.5	ng	307359	5	13.998	1107280	20.0