

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
 Data File : BF133993.D
 Acq On : 27 Jun 2023 16:11
 Operator : CG\JU
 Sample : 03337-07
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-9

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133993.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	21	rVB	1572243	2078182	86.01%	11.477%
2	2.287	29	34	43	rVB4	28734	48762	2.02%	0.269%
3	5.092	507	511	522	rVB	151696	183915	7.61%	1.016%
4	5.487	574	578	581	rBV	2210508	2030032	84.02%	11.211%
5	6.486	743	748	751	rBV	2315509	2196877	90.93%	12.132%
6	6.851	806	810	813	rBV	811148	644577	26.68%	3.560%
7	7.410	901	905	908	rBV	1400195	1247564	51.64%	6.890%
8	8.128	1024	1027	1041	rVB	998562	816334	33.79%	4.508%
9	9.204	1207	1210	1214	rBV	2730985	2416088	100.00%	13.343%
10	9.886	1323	1326	1330	rBV	1014248	810253	33.54%	4.475%
11	10.604	1444	1448	1454	rBV	181863	144973	6.00%	0.801%
12	10.680	1457	1461	1471	rBV	1548059	1331371	55.10%	7.352%
13	11.380	1576	1580	1588	rBV	902859	779229	32.25%	4.303%
14	11.910	1667	1670	1675	rBV	124167	119081	4.93%	0.658%
15	12.980	1847	1852	1855	rBV	2062316	1798490	74.44%	9.932%
16	13.557	1945	1950	1952	rBV2	24050	27467	1.14%	0.152%
17	13.886	2001	2006	2014	rBV3	152995	344883	14.27%	1.905%
18	14.039	2028	2032	2038	rVB	564606	539580	22.33%	2.980%
19	14.210	2058	2061	2066	rBV2	27162	33593	1.39%	0.186%
20	14.515	2110	2113	2115	rBV2	26397	26672	1.10%	0.147%
21	15.545	2283	2288	2293	rBV	381894	490205	20.29%	2.707%

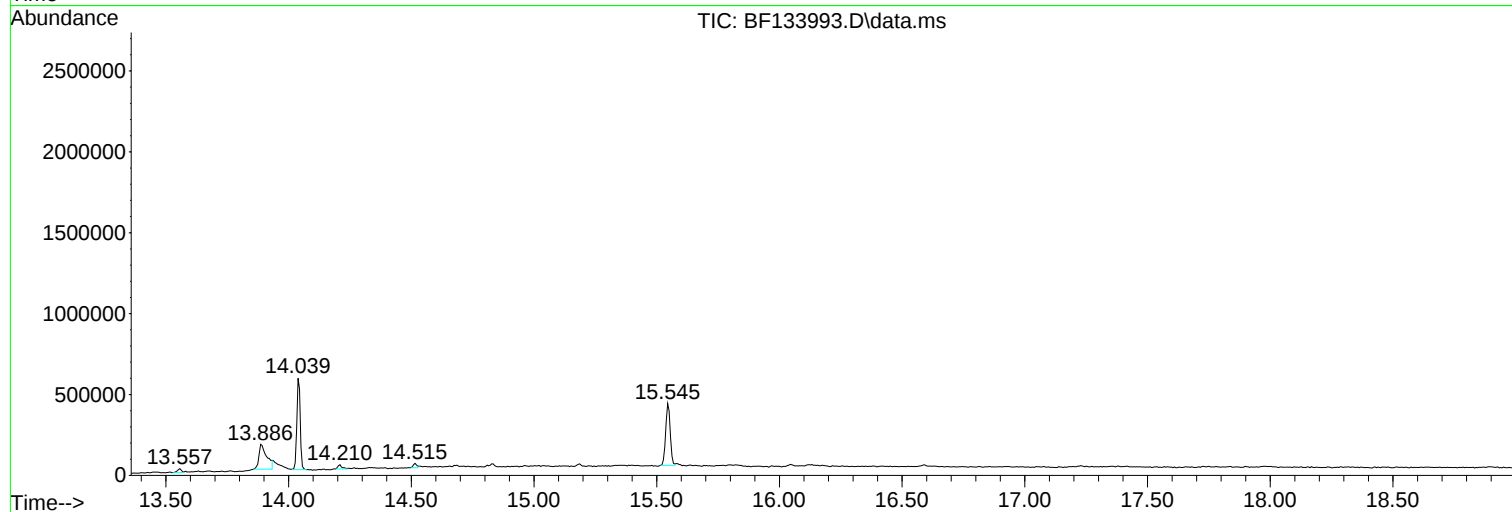
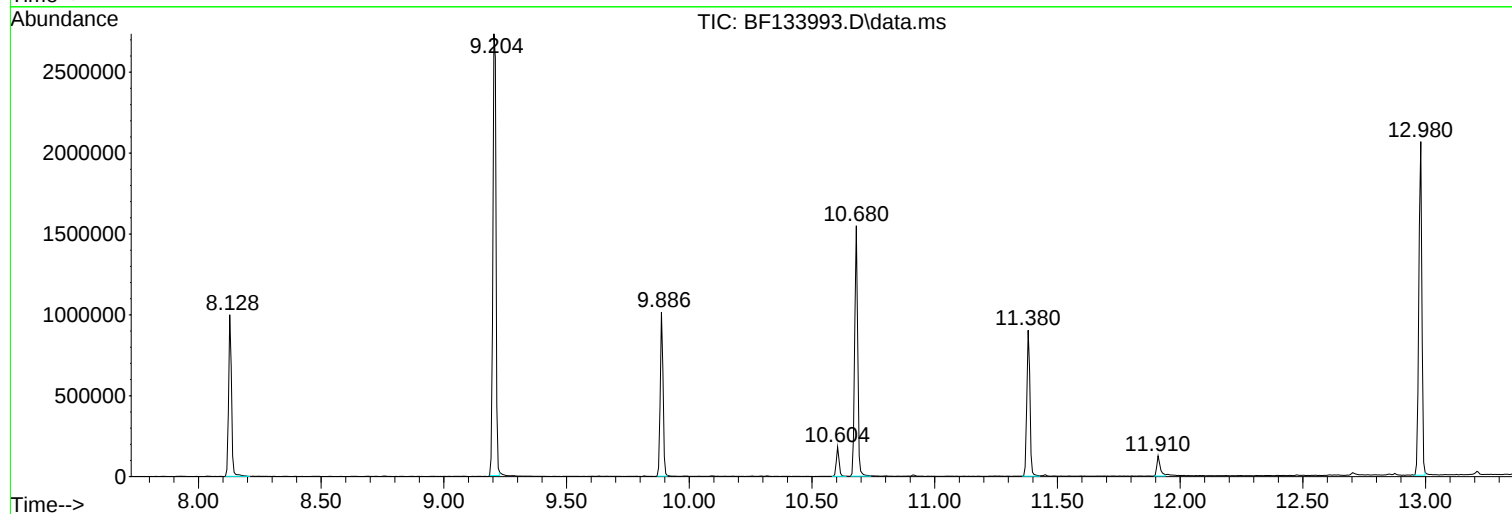
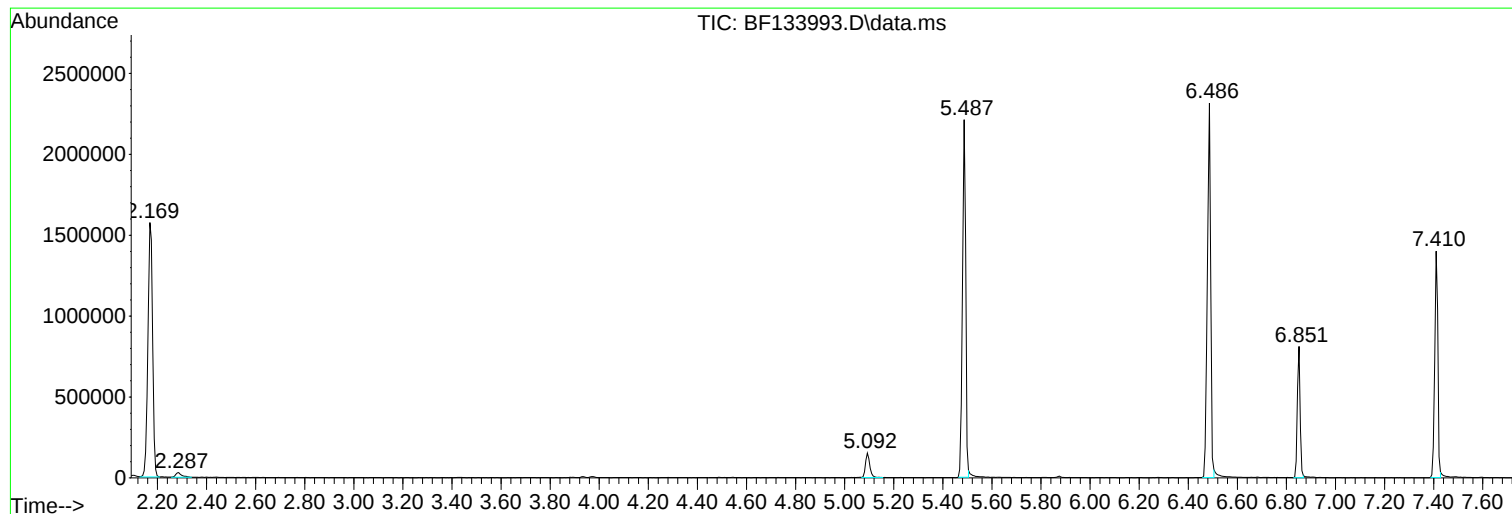
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF133993.D
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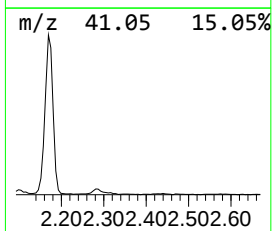
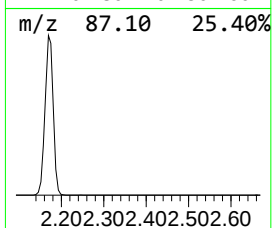
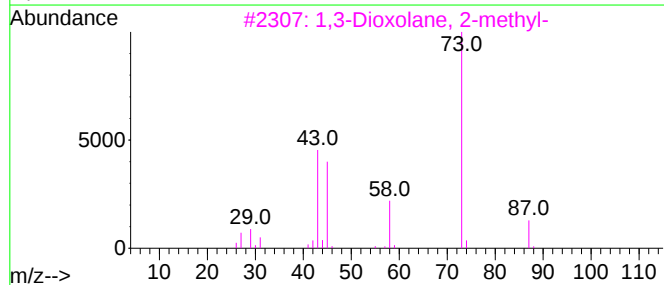
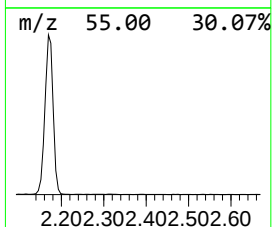
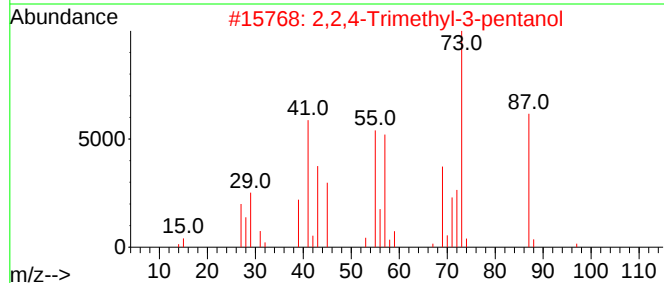
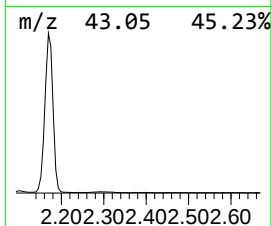
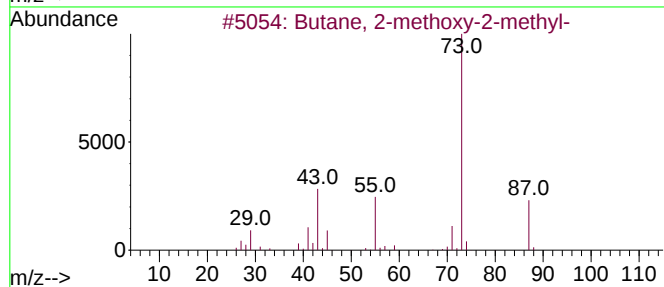
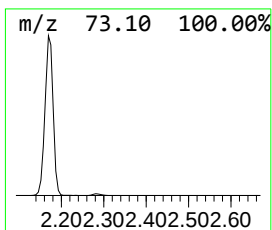
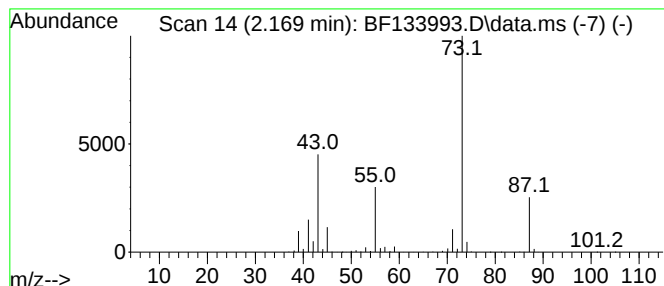
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.169	64.48 ng	2078180	1,4-Dichlorobenzene-d4	6.851

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	37
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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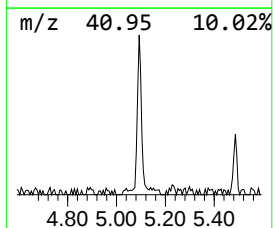
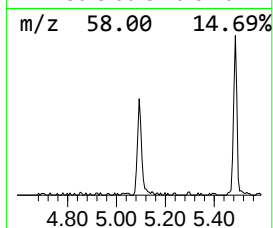
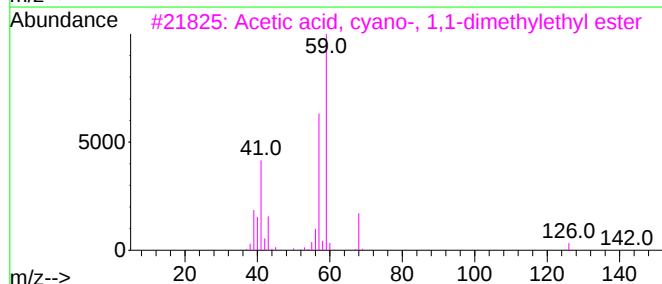
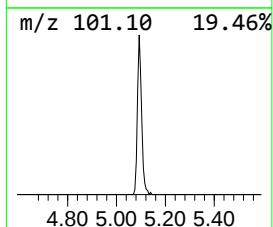
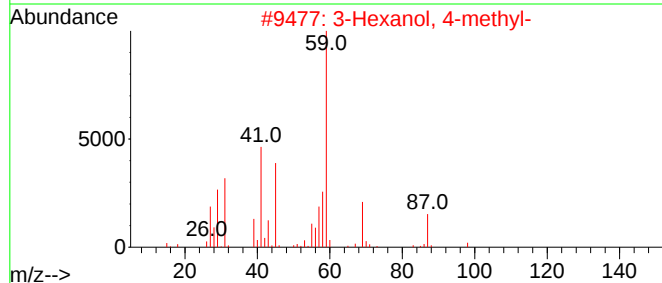
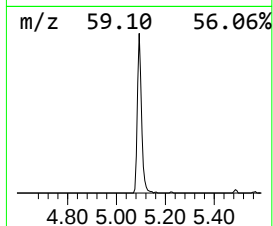
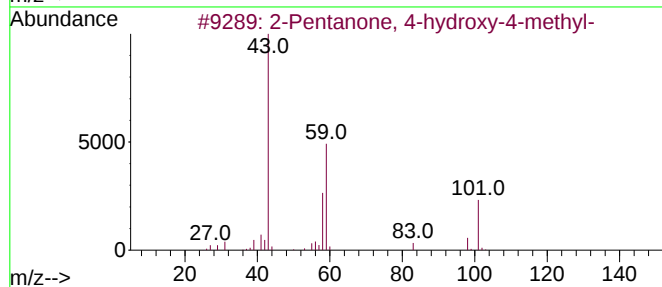
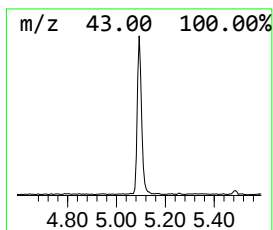
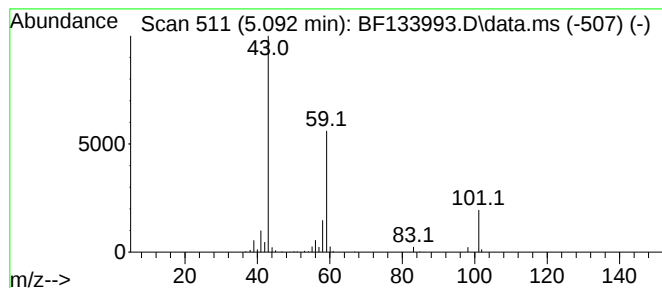
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	5.71 ng	183915	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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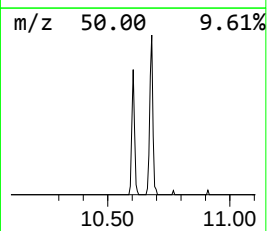
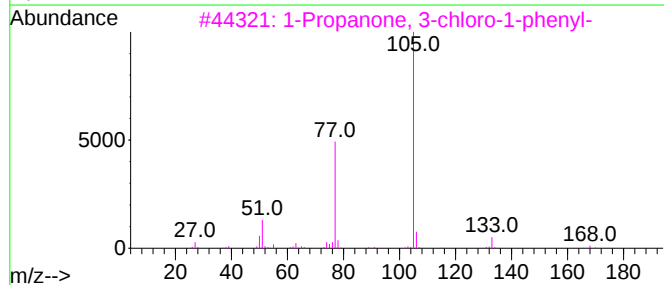
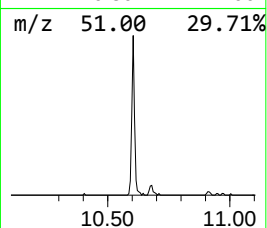
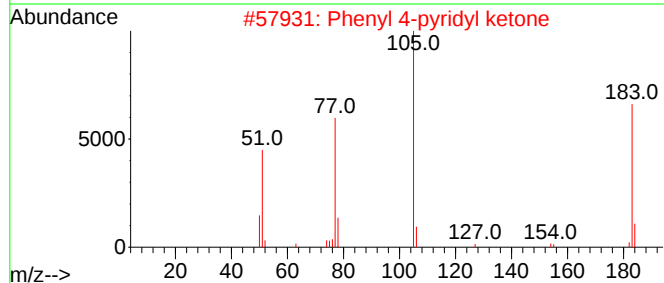
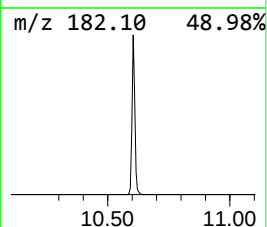
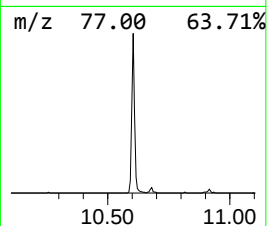
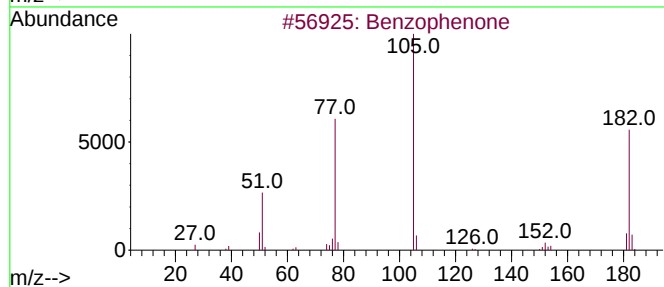
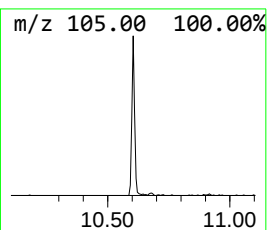
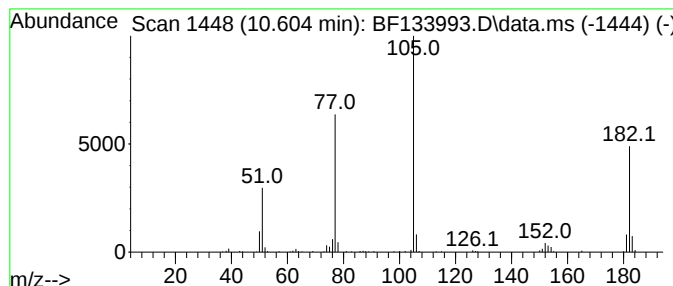
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	3.58 ng	144973	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	52
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	50
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	50
5			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50



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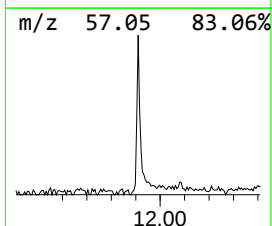
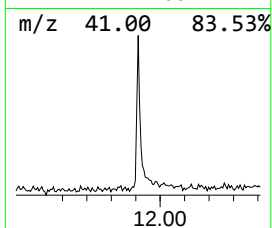
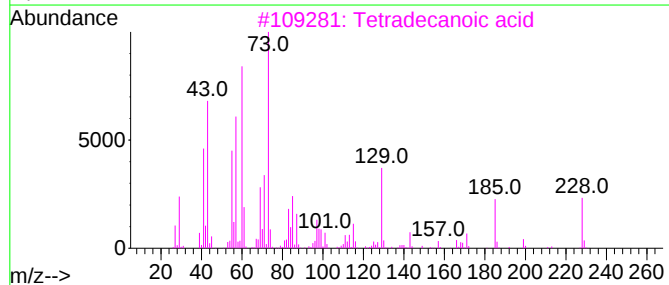
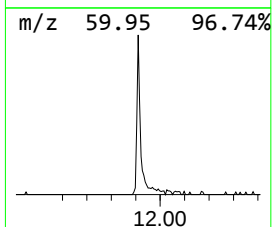
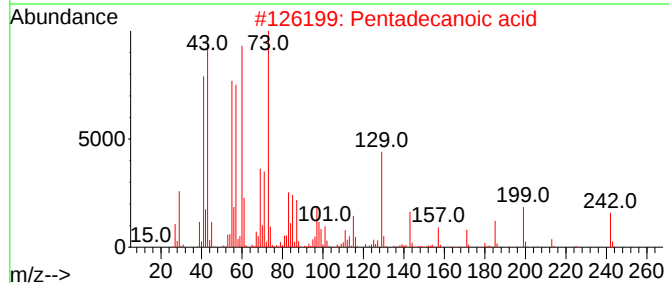
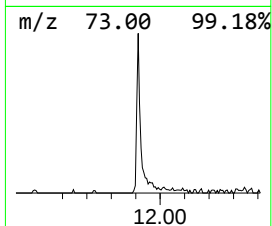
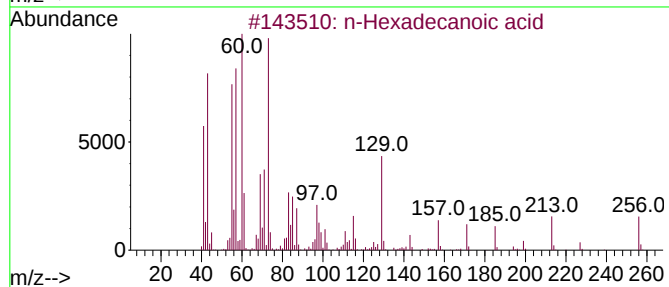
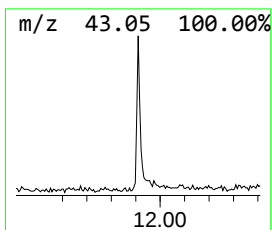
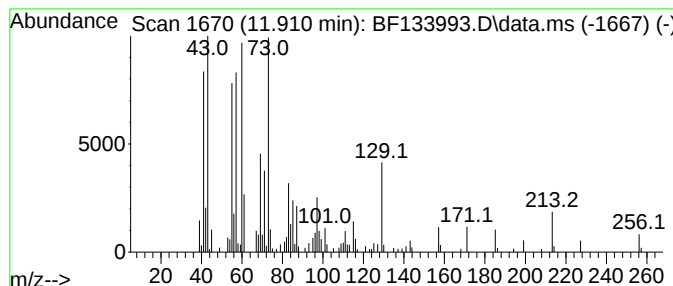
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.06 ng	119081	Phenanthrene-d10	11.380

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	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	62



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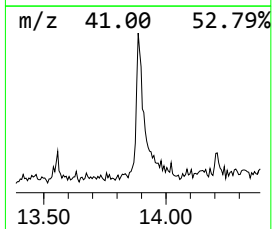
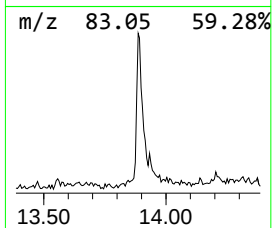
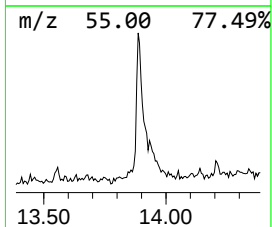
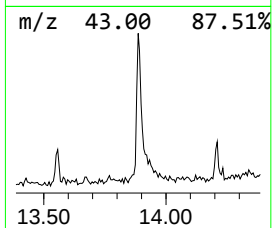
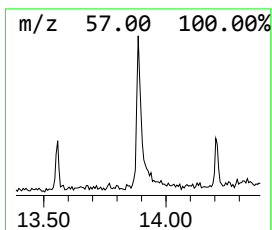
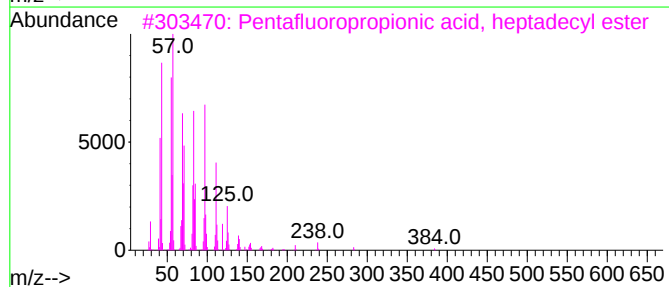
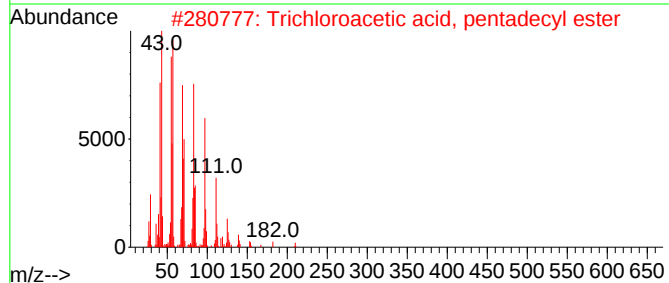
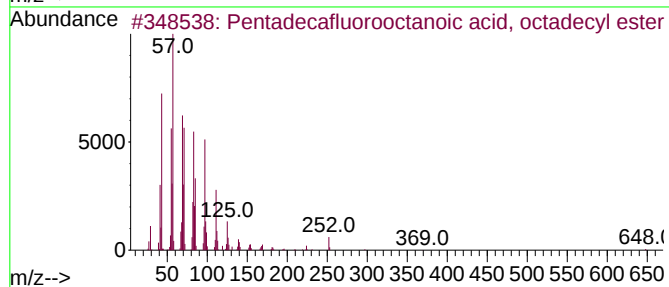
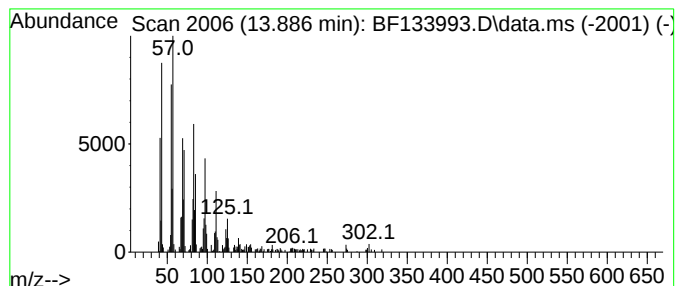
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	12.78 ng	344883	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
5			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	64.5	ng	2078180	1	6.851	644577	20.0
2-Pentanone, 4-...	5.092	5.7	ng	183915	1	6.851	644577	20.0
Benzophenone	10.604	3.6	ng	144973	3	9.886	810253	20.0
n-Hexadecanoic ...	11.910	3.1	ng	119081	4	11.380	779229	20.0
Pentadecafluoro...	13.886	12.8	ng	344883	5	14.039	539580	20.0