

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
 Data File : BG057075.D
 Acq On : 12 Apr 2023 23:01
 Operator : CG/JU
 Sample : 02283-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20230326-COMP-4

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_G\Methods\8270-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057075.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.430	315	322	329	rBV	39344	63119	4.50%	1.050%
2	5.917	398	405	418	rVB	364998	589728	42.07%	9.810%
3	7.539	673	681	692	rBV	372240	635772	45.36%	10.576%
4	8.402	818	828	836	rBV	53801	92076	6.57%	1.532%
5	9.583	1020	1029	1037	rBV	217431	380848	27.17%	6.335%
6	11.245	1305	1312	1319	rBV	70476	124980	8.92%	2.079%
7	13.642	1713	1720	1727	rBV	569482	876533	62.54%	14.580%
8	15.017	1948	1954	1963	rVB2	116297	179382	12.80%	2.984%
9	16.350	2176	2181	2187	rVB	35751	50294	3.59%	0.837%
10	16.497	2199	2206	2218	rBV	492572	743850	53.07%	12.373%
11	17.754	2412	2420	2426	rBV	158081	231007	16.48%	3.843%
12	18.588	2558	2562	2571	rBV2	28527	41751	2.98%	0.694%
13	20.321	2851	2857	2864	rBV	1053442	1401626	100.00%	23.315%
14	21.631	3075	3080	3088	rBV3	37121	64316	4.59%	1.070%
15	22.072	3149	3155	3161	rVB2	138461	238813	17.04%	3.972%
16	22.871	3285	3291	3295	rBV6	7486	14554	1.04%	0.242%
17	23.846	3453	3457	3464	rVB3	15174	30139	2.15%	0.501%
18	25.602	3744	3756	3767	rVB3	79554	252945	18.05%	4.208%

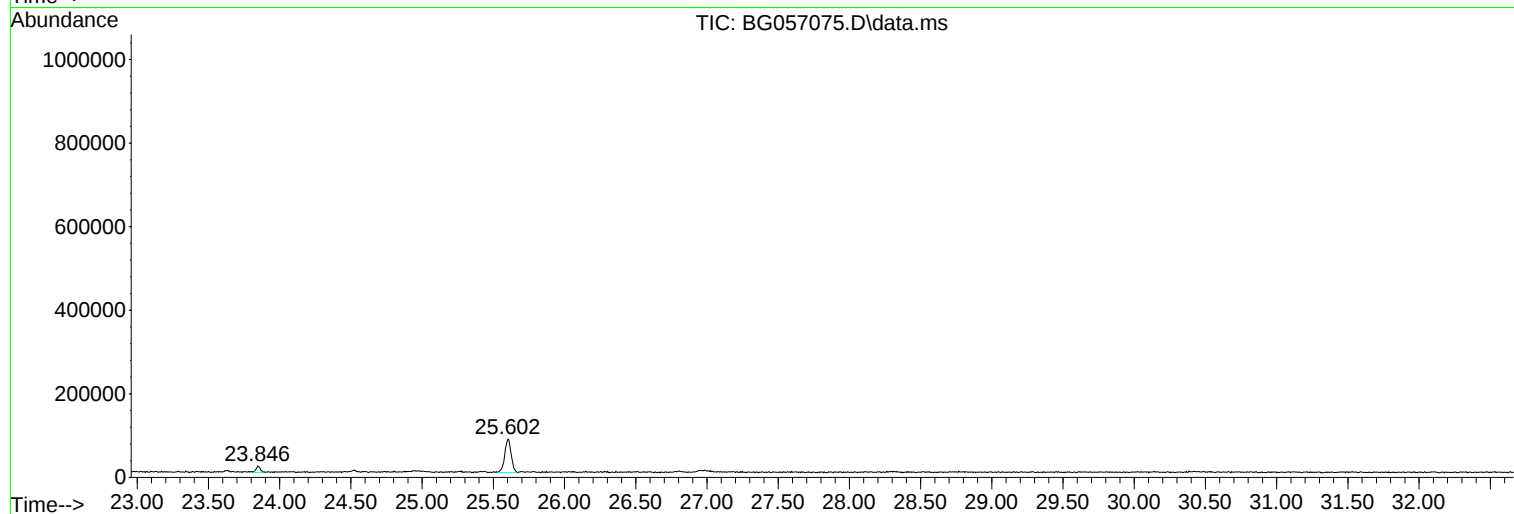
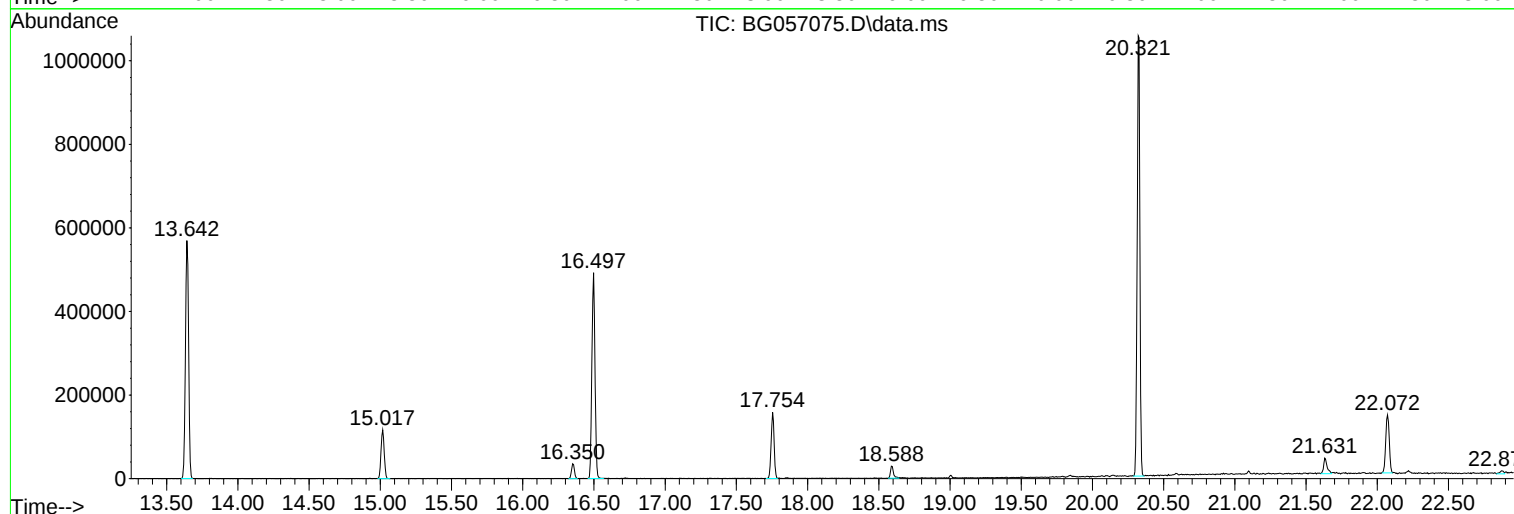
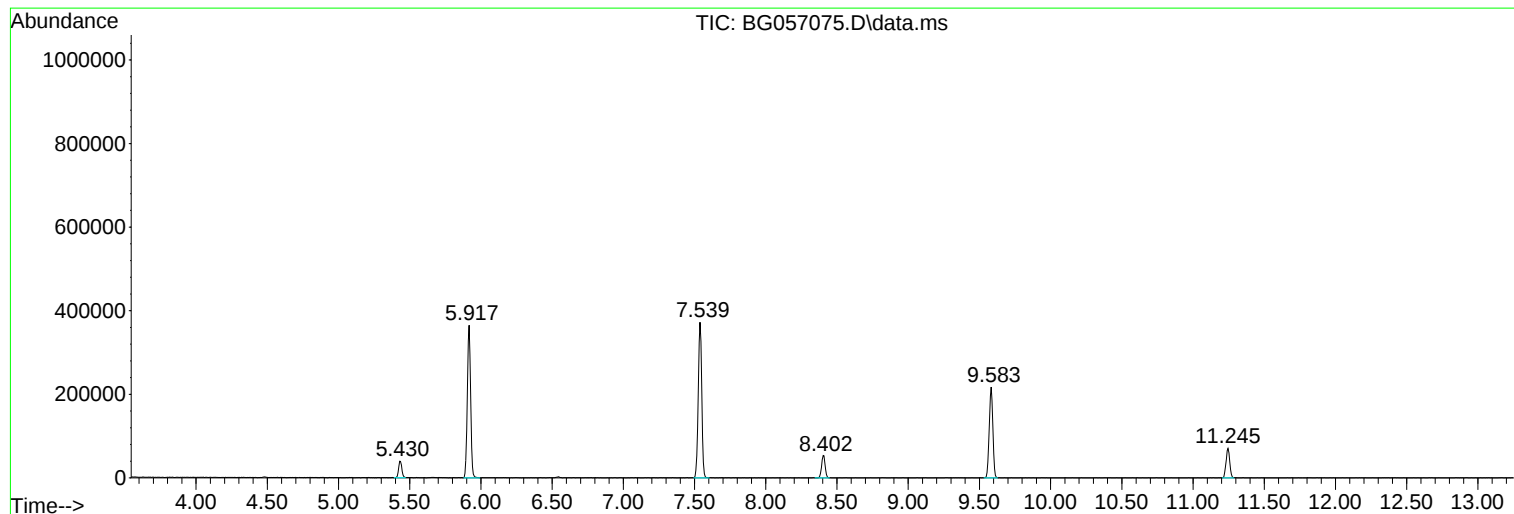
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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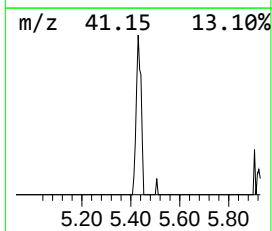
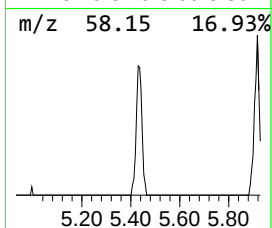
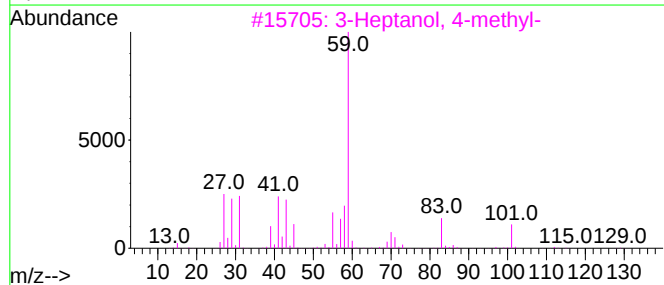
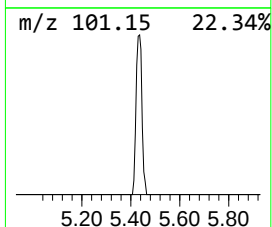
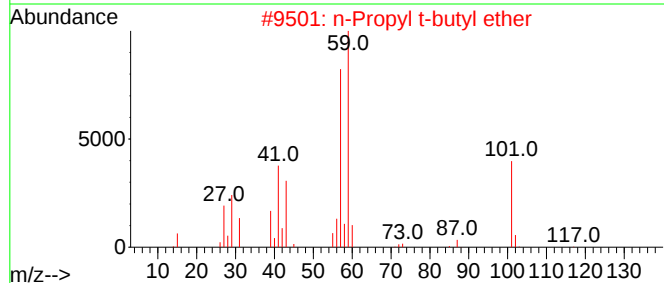
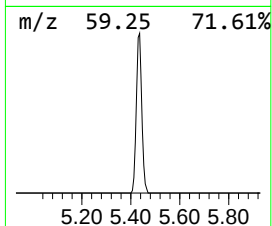
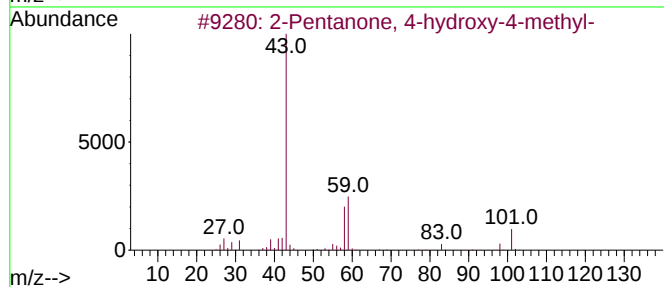
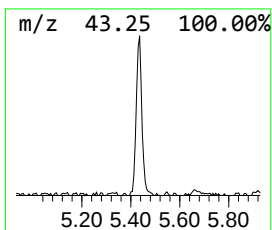
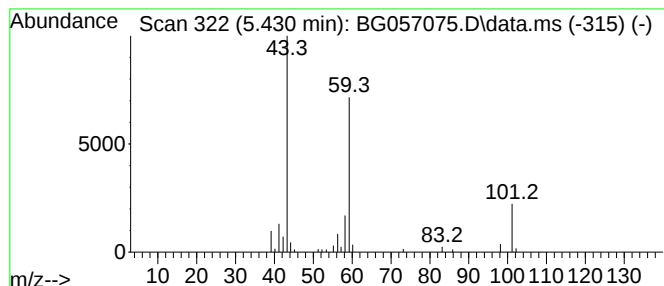
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.430	13.71 ng	63119	1,4-Dichlorobenzene-d4	8.402

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	25
4			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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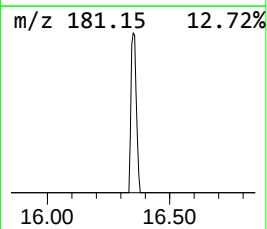
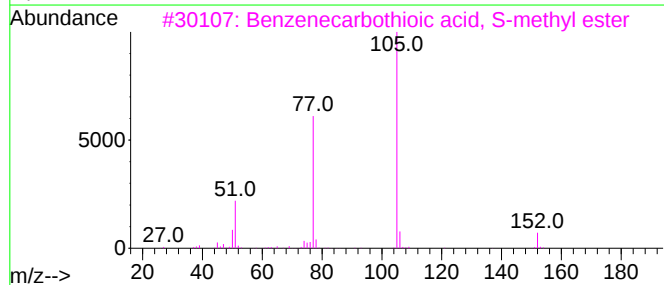
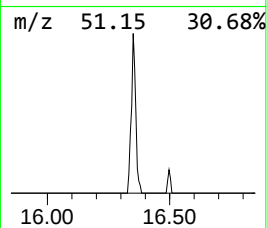
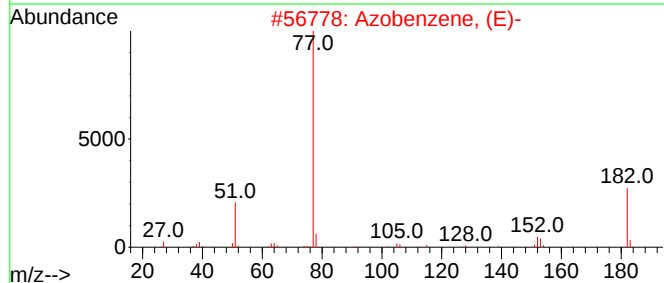
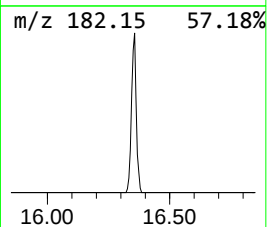
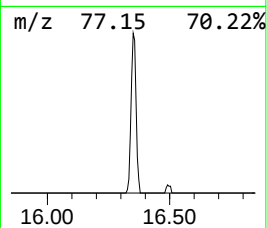
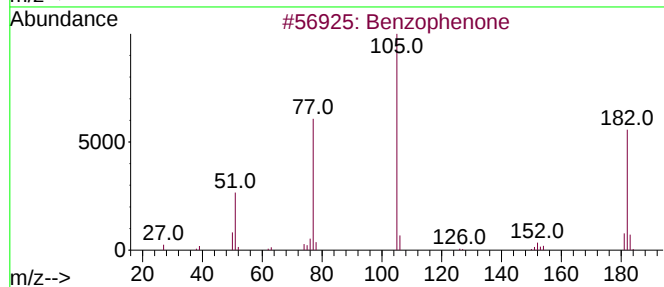
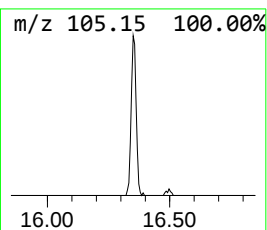
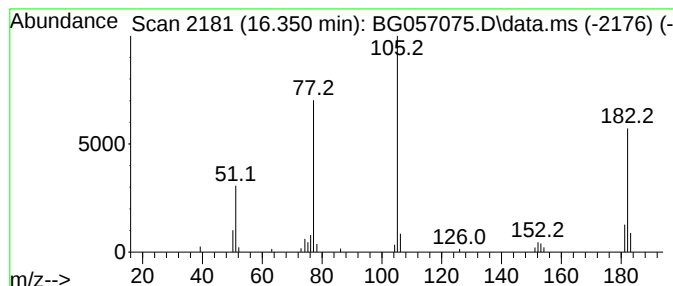
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.350	5.61 ng	50294	Acenaphthene-d10	15.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	43
5			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	43



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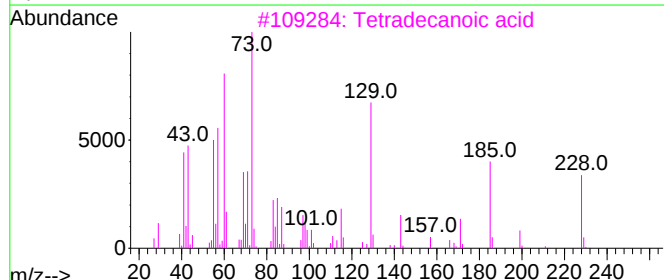
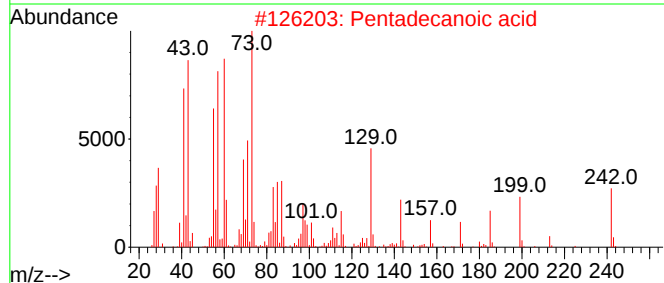
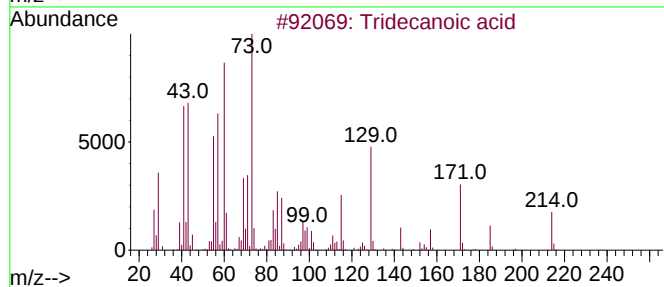
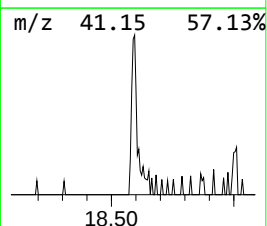
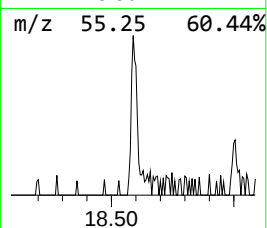
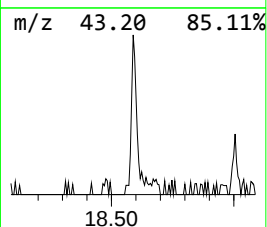
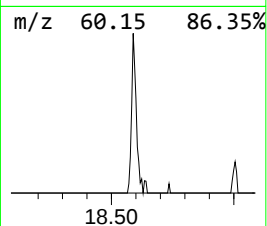
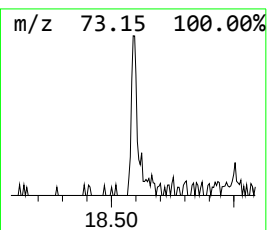
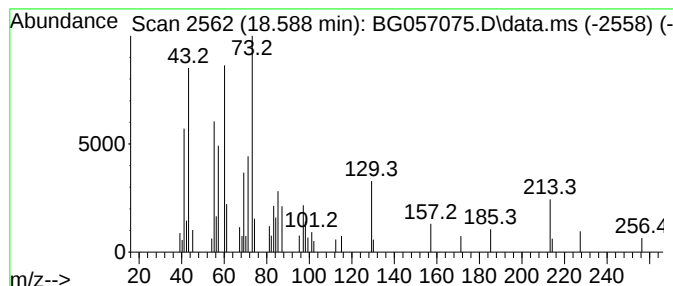
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.588	3.61 ng	41751	Phenanthrene-d10	17.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	87
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Undecanoic acid	186	C11H22O2	000112-37-8	50
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43



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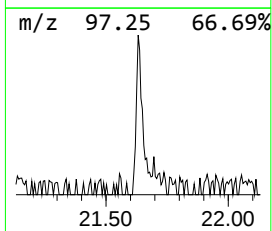
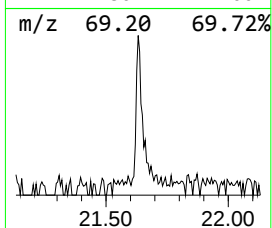
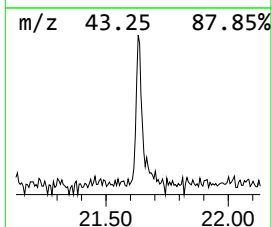
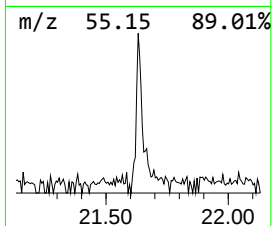
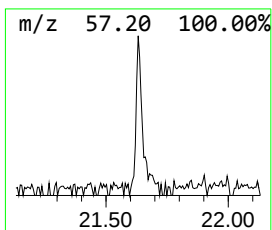
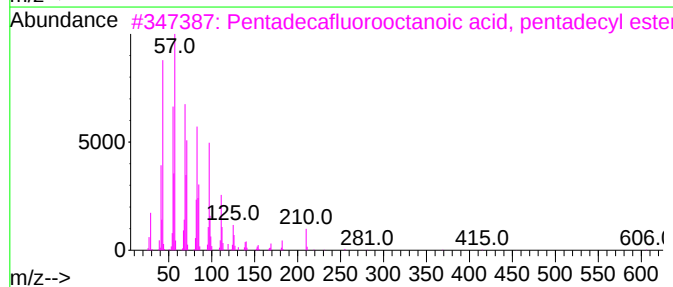
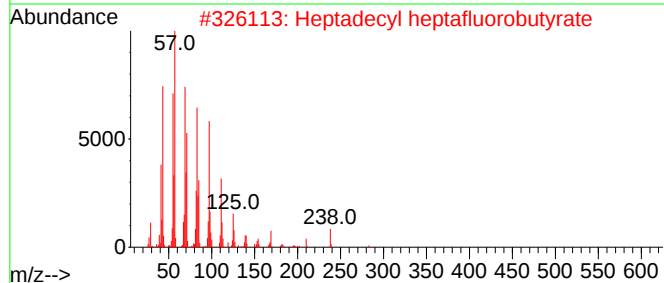
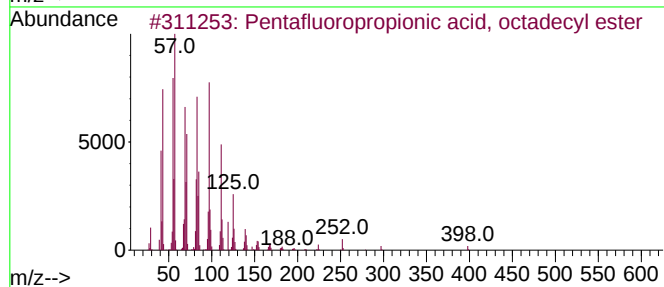
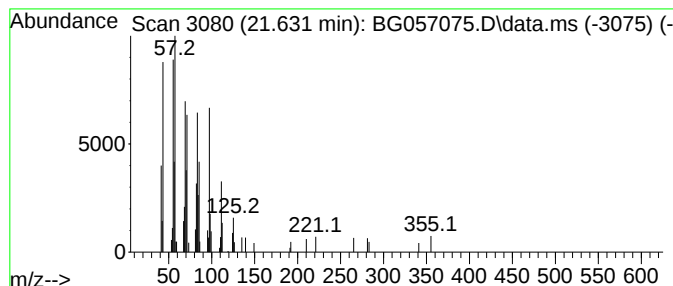
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.631	5.39 ng	64316	Chrysene-d12	22.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	91
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
5			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



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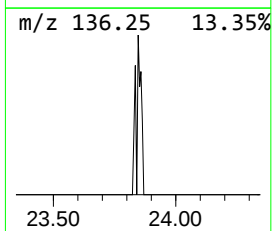
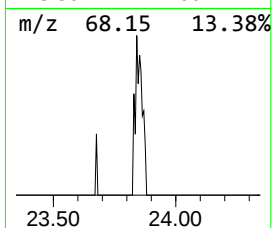
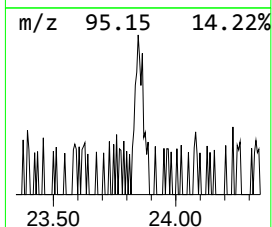
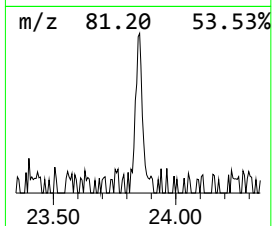
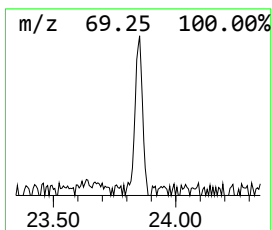
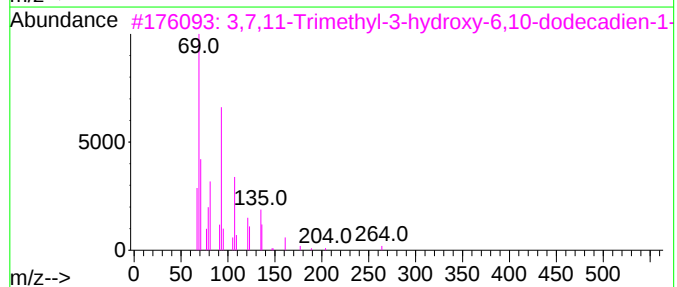
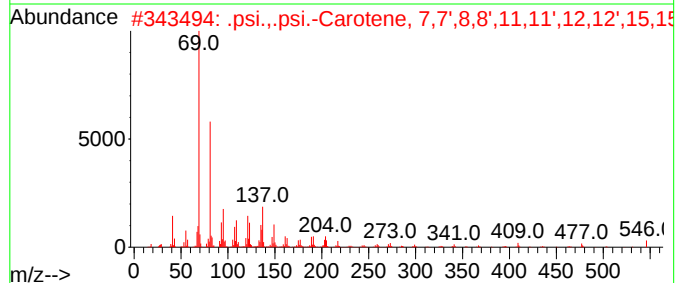
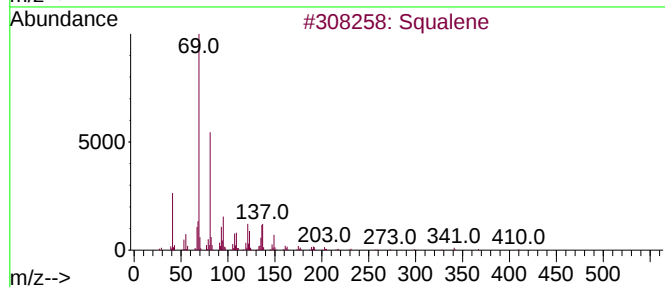
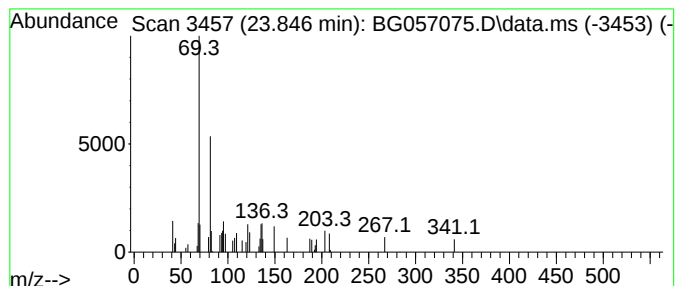
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.846	2.38 ng	30139	Perylene-d12	25.602

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	72
2			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	64
3			3,7,11-Trimethyl-3-hydroxy-6,10-...	282	C17H30O3	1000144-12-7	59
4			Propanoic acid, 2,2-dimethyl-, [...]	306	C20H34O2	1000164-38-8	59
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	59



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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
2-Pentanone, 4-...	5.430	13.7	ng	63119	1	8.402	92076	20.0
Benzophenone	16.350	5.6	ng	50294	3	15.017	179382	20.0
Tridecanoic acid	18.588	3.6	ng	41751	4	17.754	231007	20.0
Pentafluoroprop...	21.631	5.4	ng	64316	5	22.072	238813	20.0
Squalene	23.846	2.4	ng	30139	6	25.602	252945	20.0