

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
 Data File : BG055085.D
 Acq On : 6 Oct 2022 16:51
 Operator : CG/JU
 Sample : N5009-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 006-3

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-BG100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055085.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.372	9	14	42	rVB	740295	1439293	48.53%	10.170%
2	5.388	350	357	371	rVB	46089	81887	2.76%	0.579%
3	5.858	430	437	452	rBV	214266	383442	12.93%	2.709%
4	7.462	702	710	723	rVB	139254	244400	8.24%	1.727%
5	8.337	852	859	868	rBV	102050	179114	6.04%	1.266%
6	9.506	1050	1058	1067	rBV	349836	620434	20.92%	4.384%
7	11.169	1333	1341	1348	rBV	138646	250651	8.45%	1.771%
8	13.572	1743	1750	1757	rVB	900863	1405740	47.40%	9.933%
9	14.941	1977	1983	1990	rVB	237784	362942	12.24%	2.565%
10	16.416	2227	2234	2243	rVB	915013	1371038	46.23%	9.688%
11	17.673	2442	2448	2455	rBV	347546	532563	17.96%	3.763%
12	18.531	2589	2594	2602	rBV2	19346	39005	1.32%	0.276%
13	18.613	2602	2608	2614	rVV	2133879	2858838	96.39%	20.201%
14	20.053	2848	2853	2862	rVB	55421	72598	2.45%	0.513%
15	20.253	2881	2887	2893	rBV	2271803	2965857	100.00%	20.957%
16	21.569	3107	3111	3121	rVB2	38467	65531	2.21%	0.463%
17	21.968	3172	3179	3189	rVB	377484	638767	21.54%	4.514%
18	25.417	3756	3766	3779	rBV2	210536	640029	21.58%	4.522%

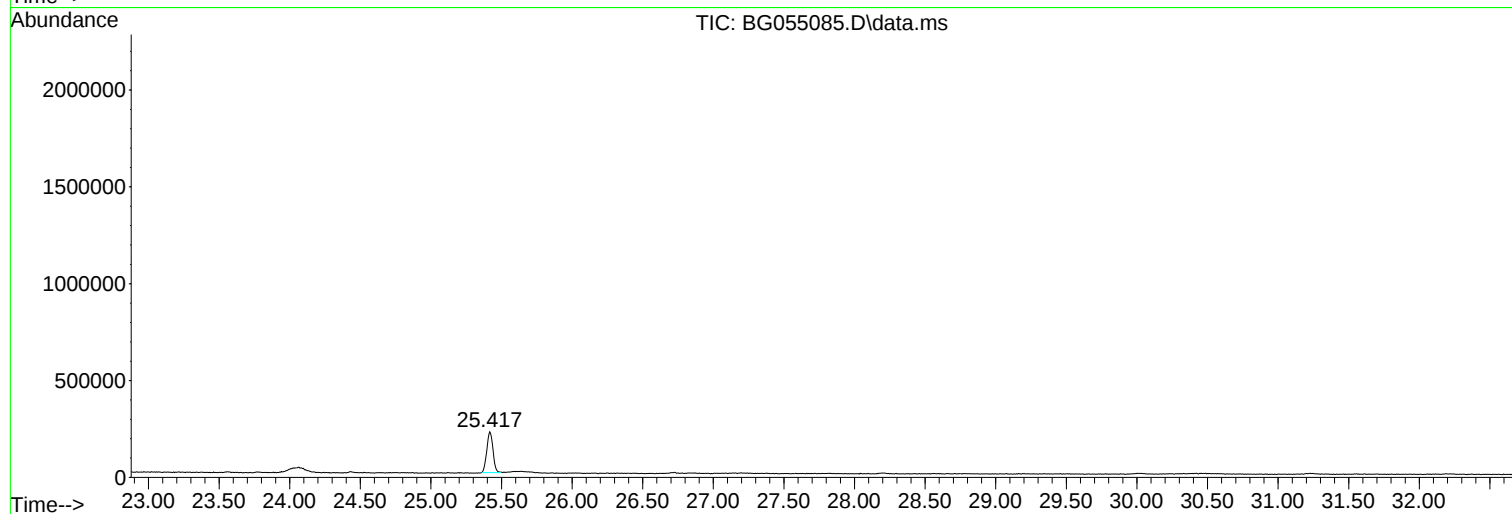
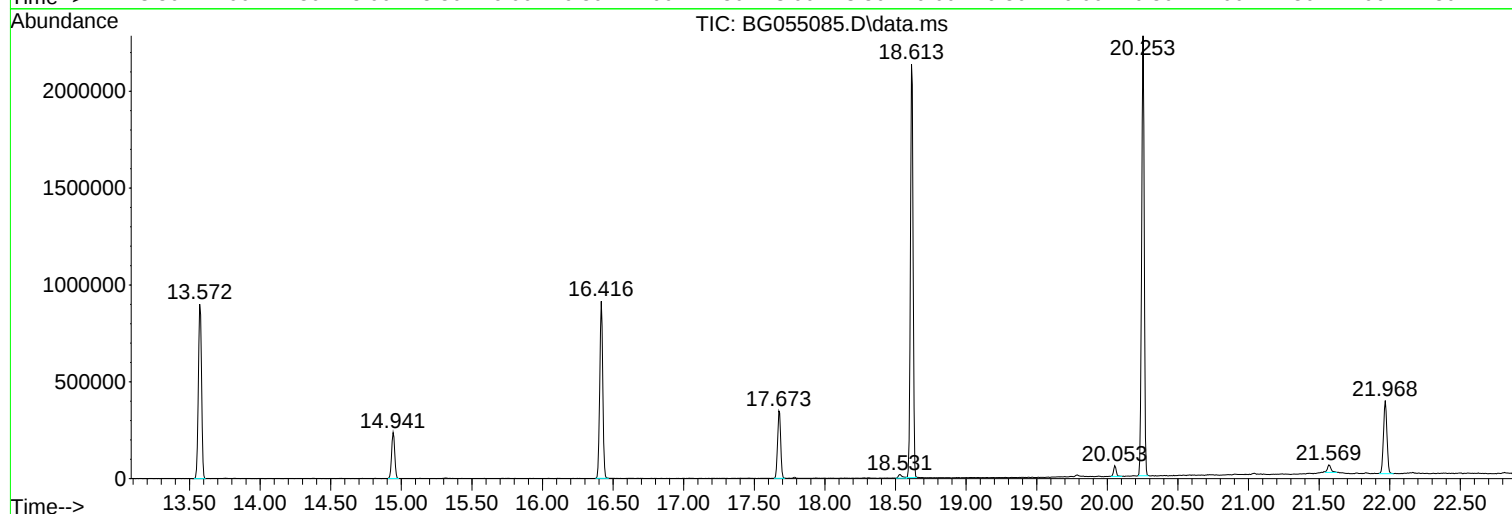
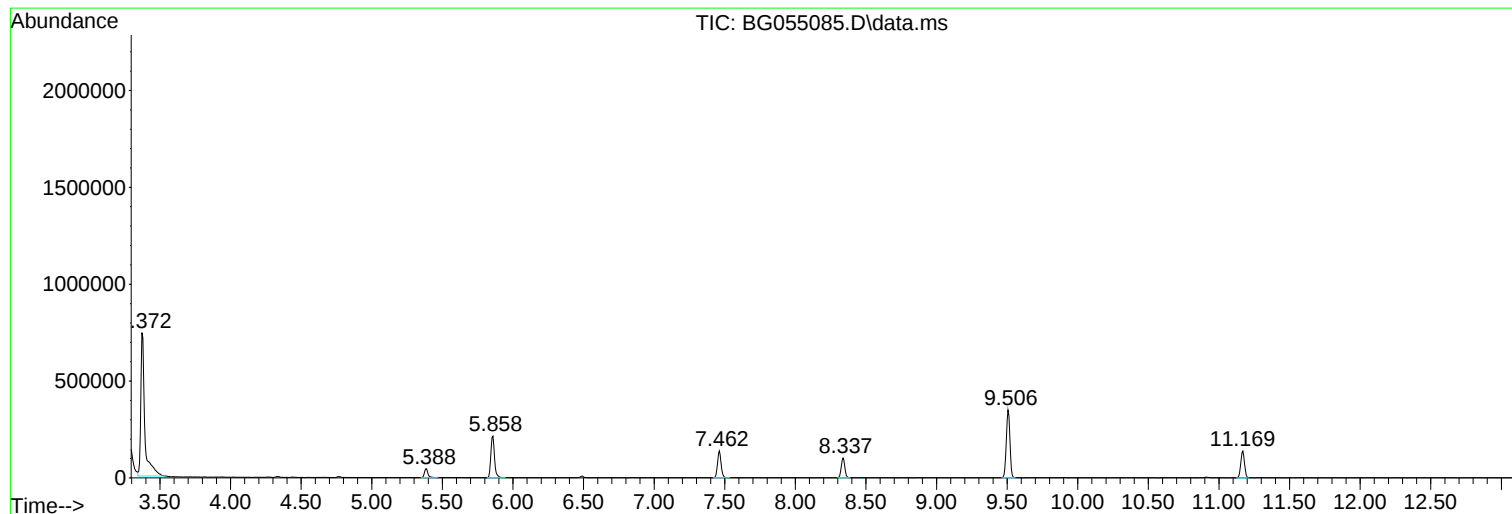
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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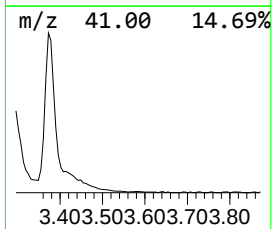
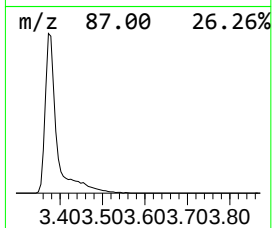
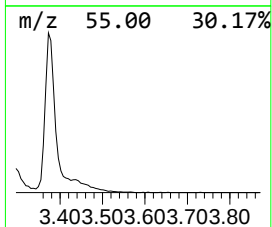
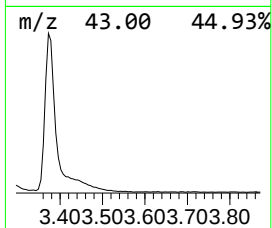
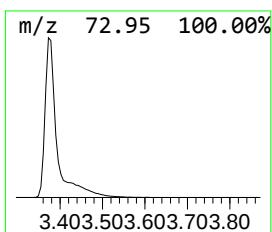
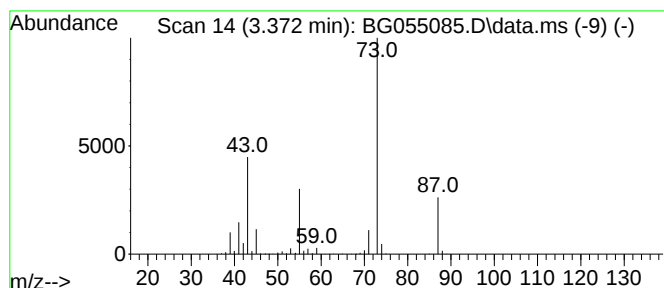
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.372	160.71 ng	1439290	1,4-Dichlorobenzene-d4	8.337

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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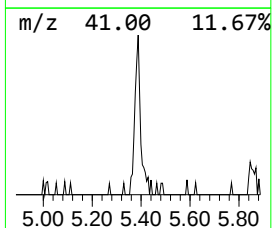
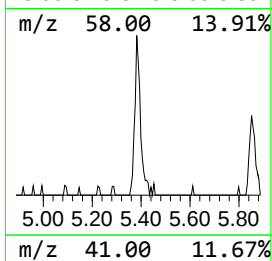
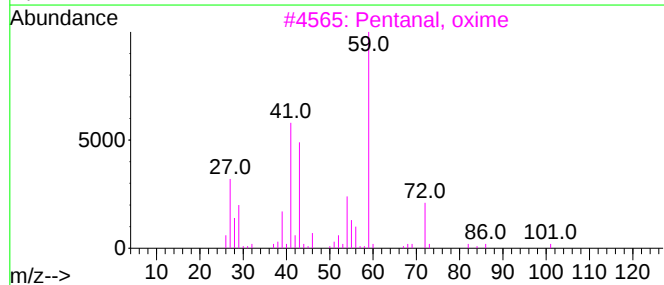
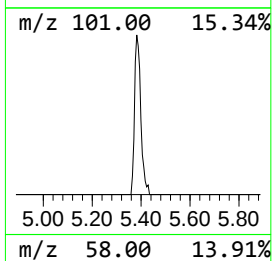
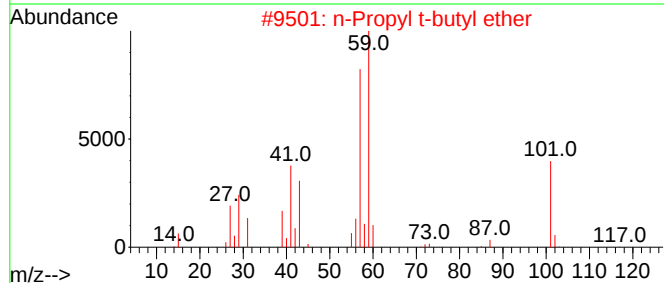
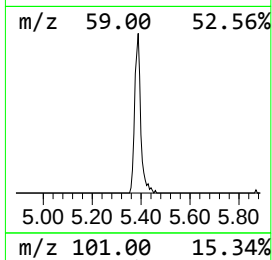
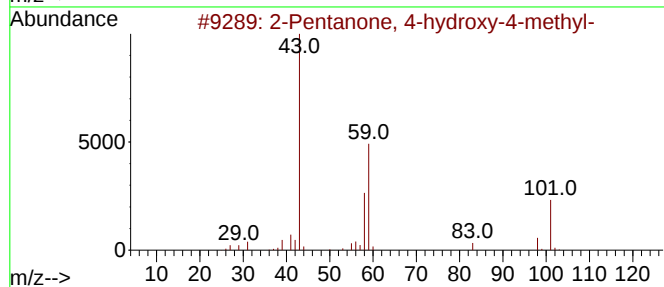
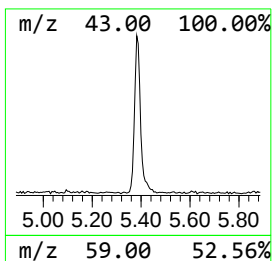
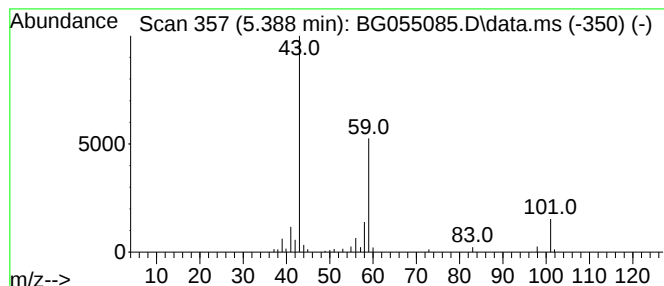
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.388	9.14 ng	81887	1,4-Dichlorobenzene-d4	8.337

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			Pentanal, oxime	101	C5H11NO	000628-79-5	25
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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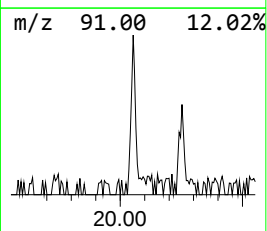
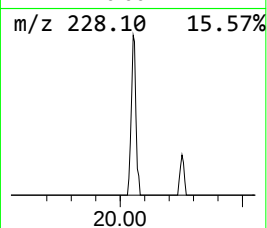
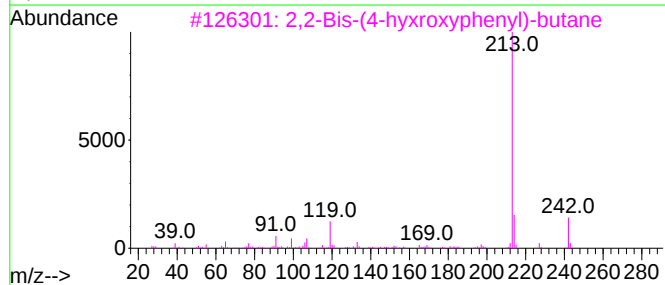
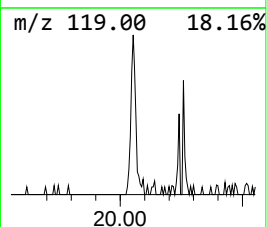
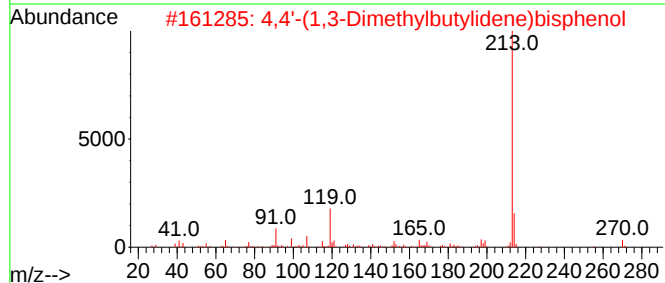
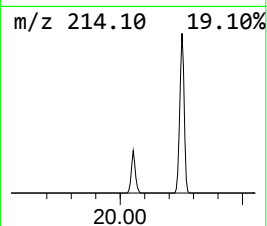
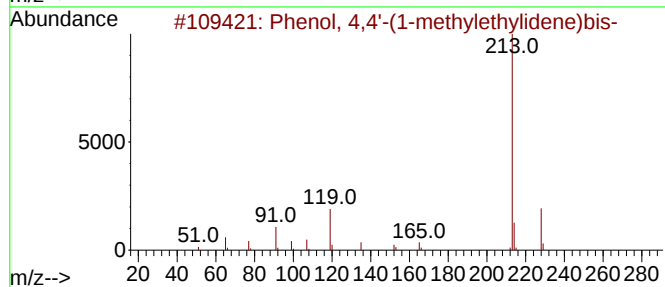
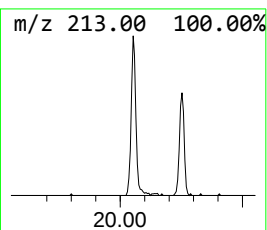
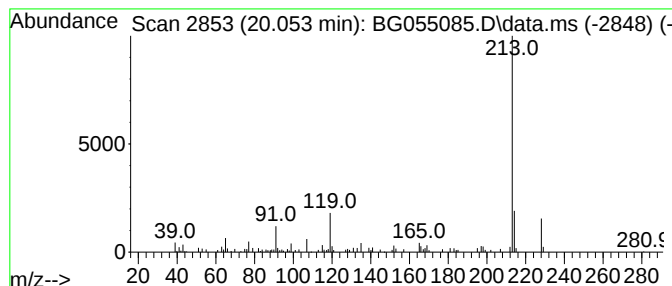
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Peak Number 3 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.053	2.27 ng	72598	Chrysene-d12	21.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	95
2			4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	87
3			2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	59
4			Diphenolic acid	286	C17H18O4	000126-00-1	50
5			2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	50



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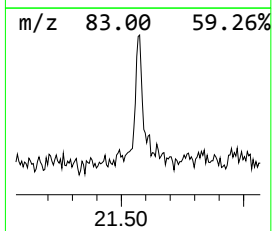
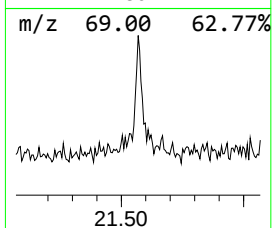
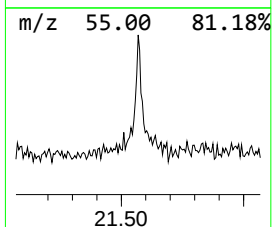
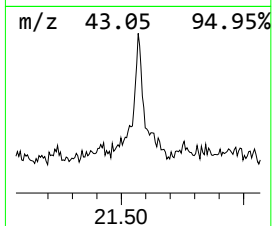
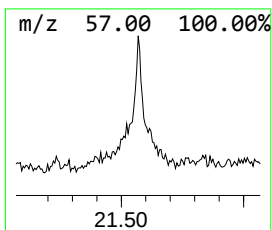
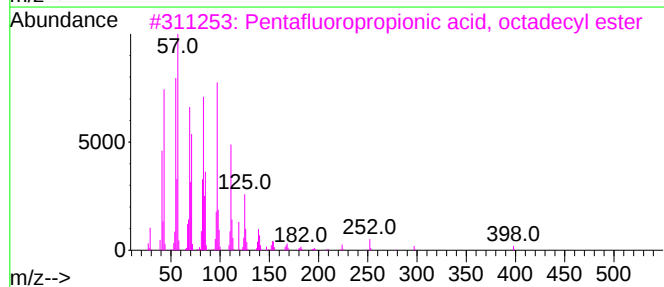
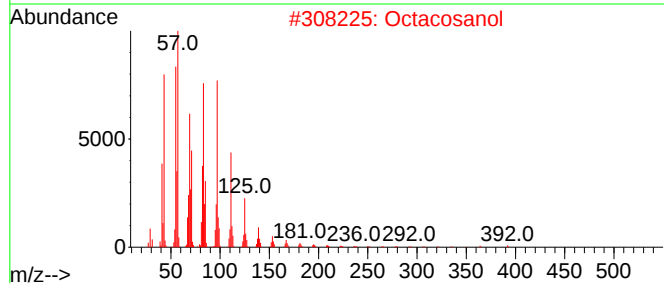
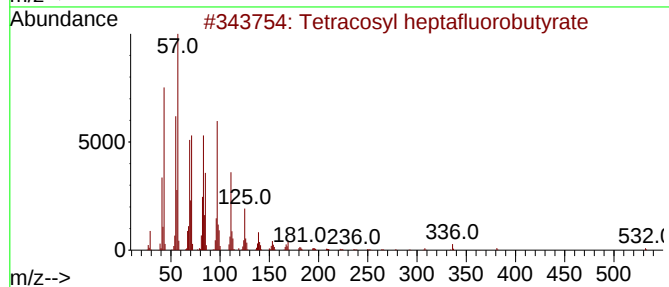
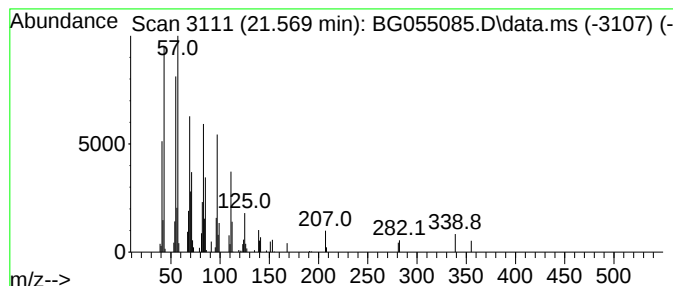
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Peak Number 4 Tetracosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.569	2.05 ng	65531	Chrysene-d12		21.968	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetracosyl heptafluorobutyrate		550	C28H49F7O2	1000351-83-7	81
2	Octacosanol		410	C28H58O	000557-61-9	76
3	Pentafluoropropionic acid, octadecyl ester		416	C21H37F5O2	959261-25-7	74
4	Triacontan-15-ol		438	C30H62O	031849-26-0	74
5	Octacosyl trifluoroacetate		506	C30H57F3O2	1000351-74-9	74



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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...	3.372	160.7	ng	1439290	1	8.337	179114	20.0
2-Pentanone, 4-...	5.388	9.1	ng	81887	1	8.337	179114	20.0
Phenol, 4,4'-(1...	20.053	2.3	ng	72598	5	21.968	638767	20.0
Tetracosyl hept...	21.569	2.0	ng	65531	5	21.968	638767	20.0