

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060921\
 Data File : BP005821.D
 Acq On : 09 Jun 2021 22:01
 Operator : CG/JU
 Sample : M2612-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 18-B12(26-30)

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_P\Methods\8270E-BP060821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005821.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.122	4	6	16	rVB	41264	52401	1.27%	0.281%
2	5.052	328	334	343	rVB2	55538	87948	2.14%	0.471%
3	5.516	406	413	428	rBV	1200337	1778437	43.19%	9.528%
4	7.116	677	685	702	rVB	1096101	1728306	41.97%	9.260%
5	7.952	820	827	834	rBV	236525	370617	9.00%	1.986%
6	9.116	1017	1025	1036	rBV	622967	1017125	24.70%	5.449%
7	10.757	1297	1304	1314	rBV	270633	470774	11.43%	2.522%
8	13.034	1684	1691	1708	rBV	66639	201964	4.91%	1.082%
9	13.204	1713	1720	1733	rVB	1536358	2301423	55.89%	12.330%
10	14.034	1847	1861	1875	rBV	296269	455292	11.06%	2.439%
11	14.575	1946	1953	1963	rBV	408701	615857	14.96%	3.300%
12	16.063	2199	2206	2222	rBV	1208677	1810970	43.98%	9.702%
13	17.322	2413	2420	2430	rBV	533240	764328	18.56%	4.095%
14	19.869	2847	2853	2861	rBV	3236148	4117511	100.00%	22.060%
15	21.092	3057	3061	3071	rBV	352946	540339	13.12%	2.895%
16	21.386	3106	3111	3117	rBV	835468	1070265	25.99%	5.734%
17	23.804	3516	3522	3532	rBV2	601776	1281504	31.12%	6.866%

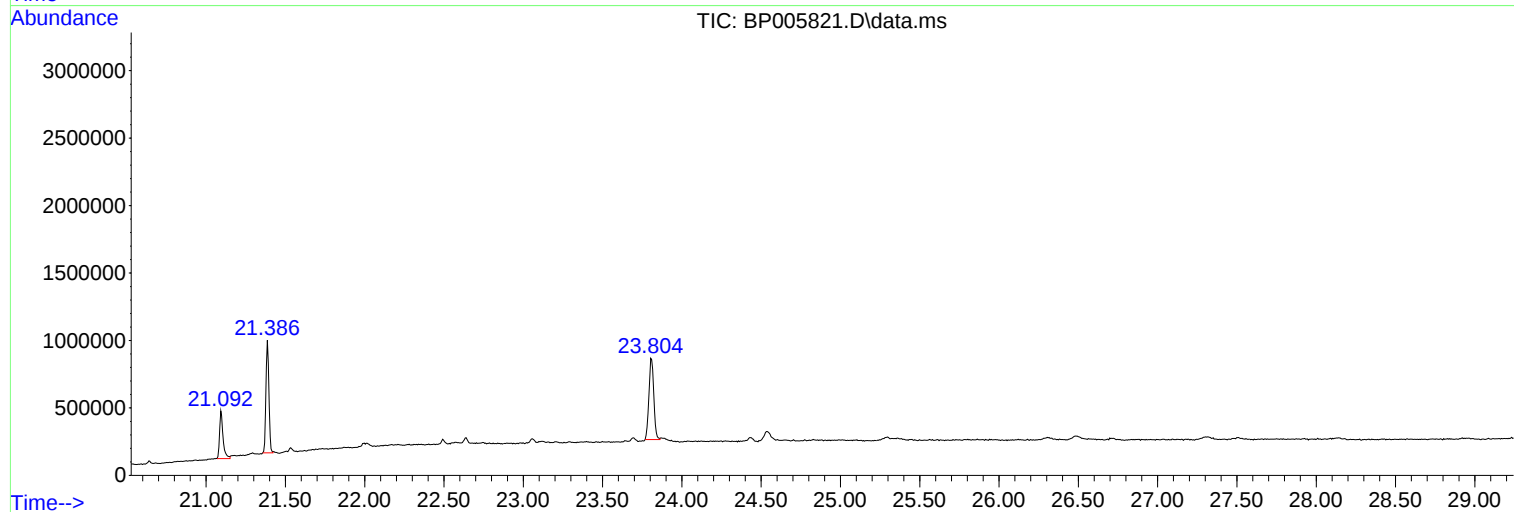
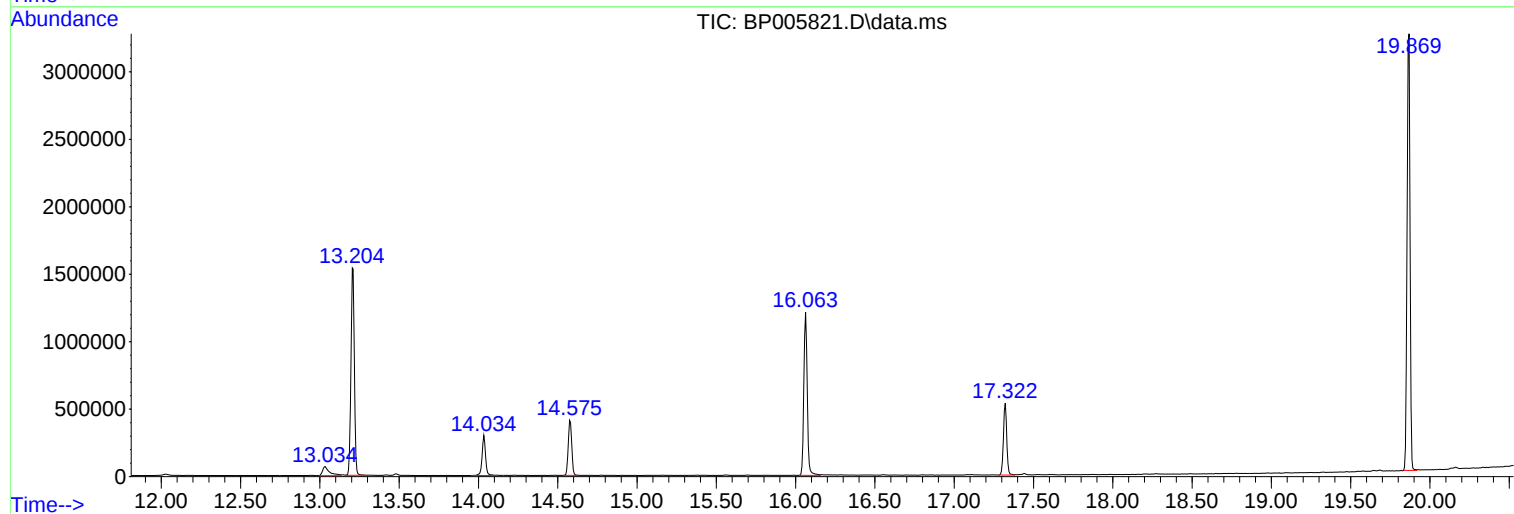
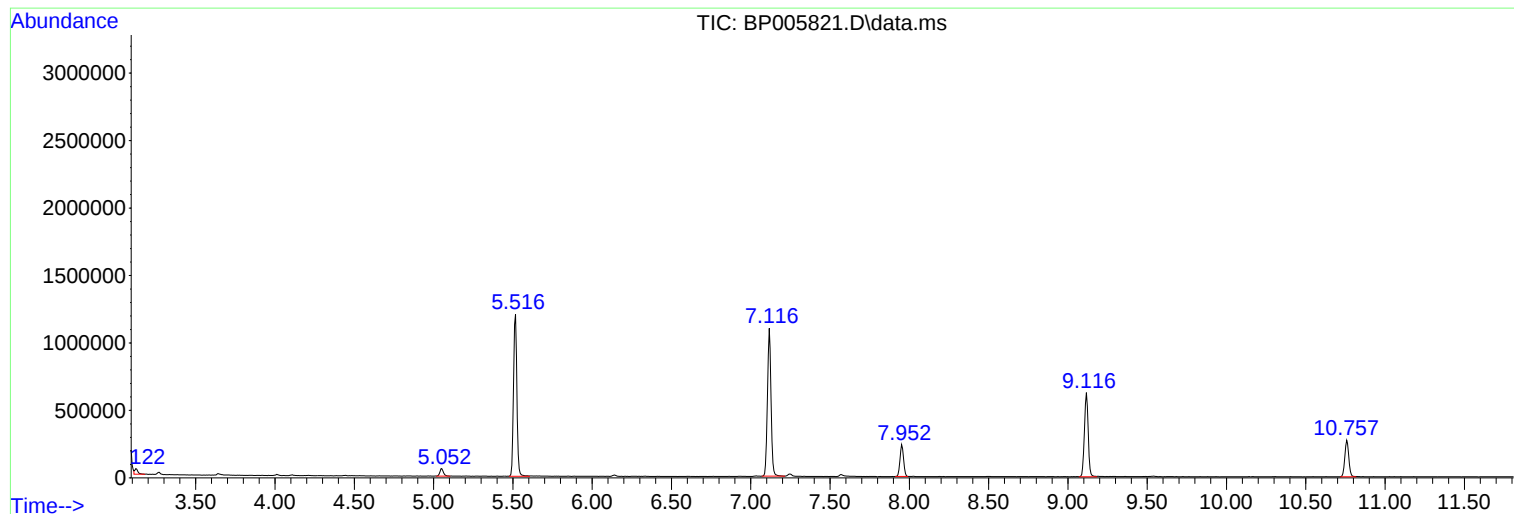
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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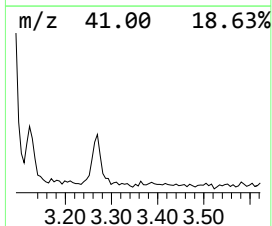
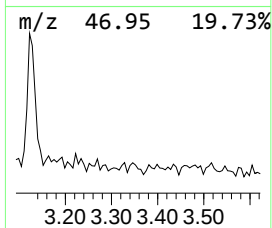
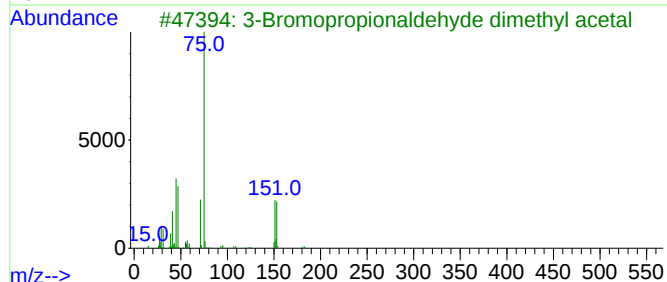
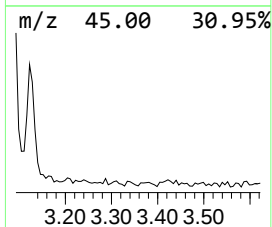
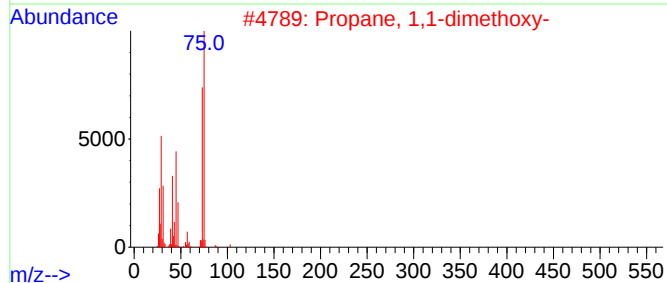
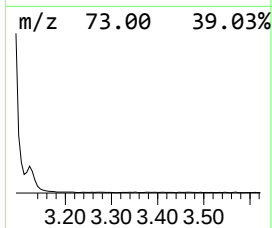
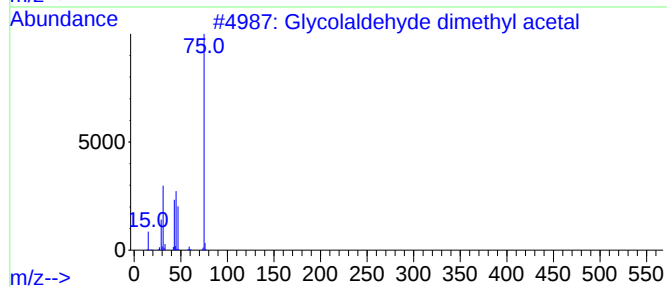
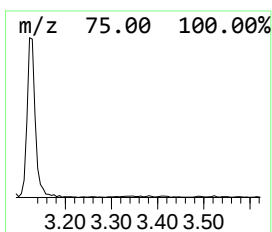
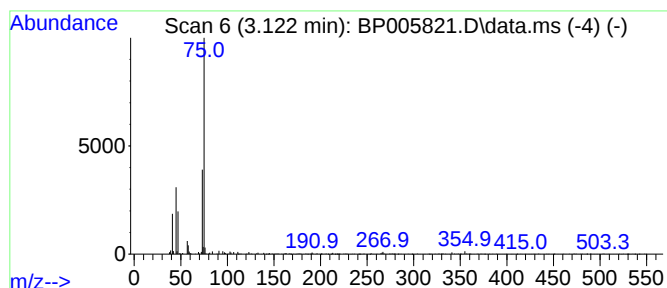
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.122 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.122	2.83 ng	52401	1,4-Dichlorobenzene-d4	7.952

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	39
2			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	39
3			3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	36
4			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	36
5			Dodecane, 1,1-dimethoxy-	230	C14H30O2	014620-52-1	25



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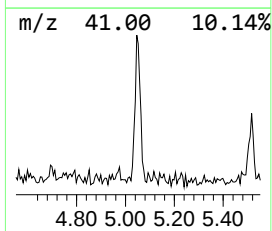
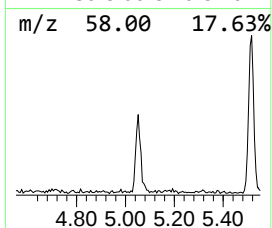
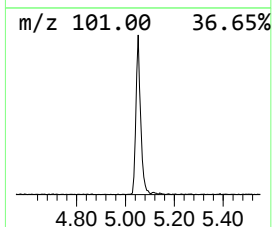
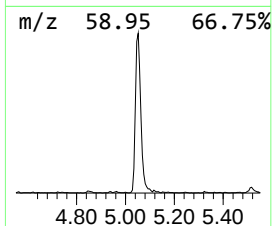
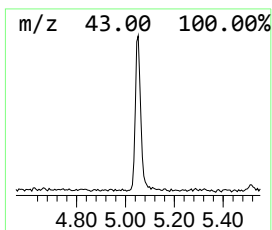
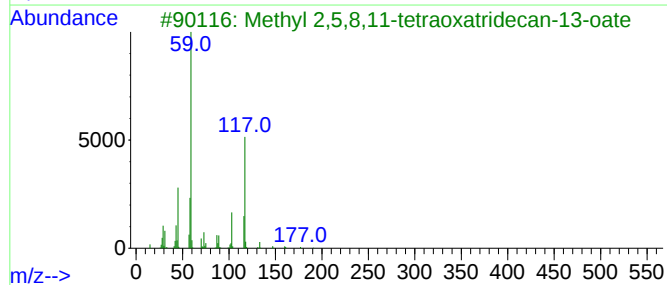
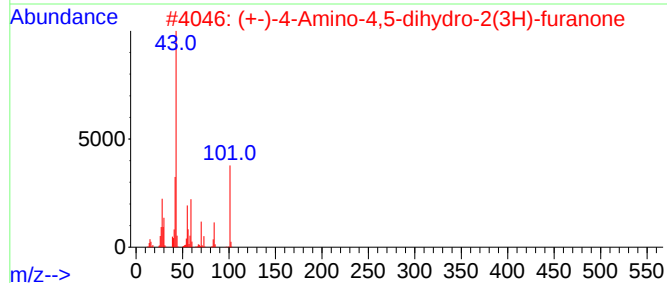
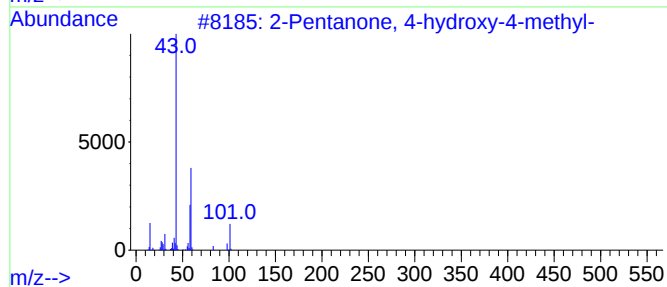
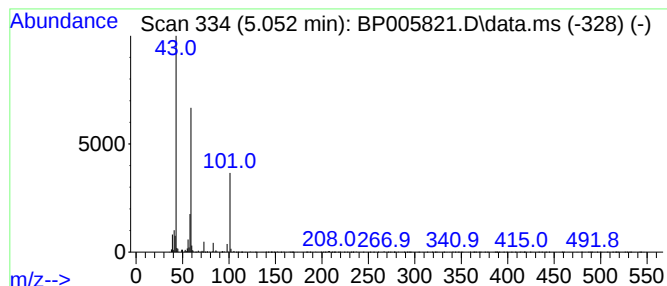
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.052	4.75 ng	87948	1,4-Dichlorobenzene-d4	7.952

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	33
3			Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	32
4			Butanoic acid, 3-hydroxy-3-methy...	132	C6H12O3	006149-45-7	28
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	27



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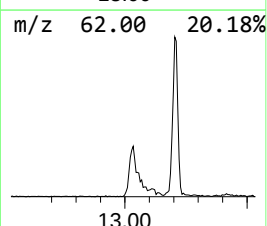
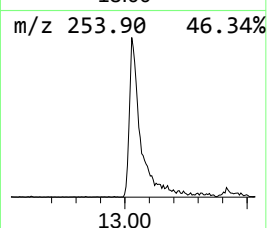
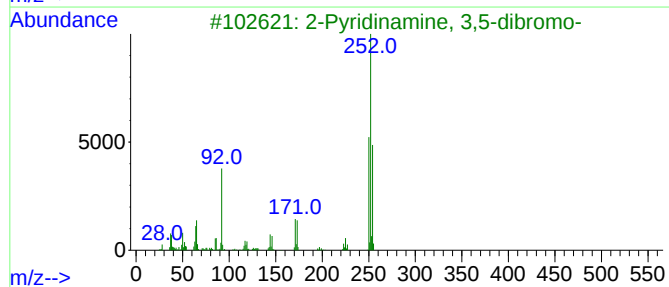
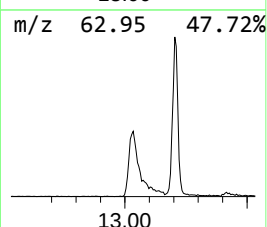
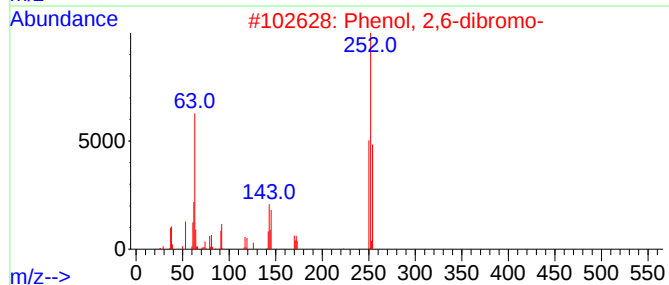
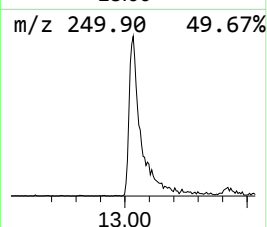
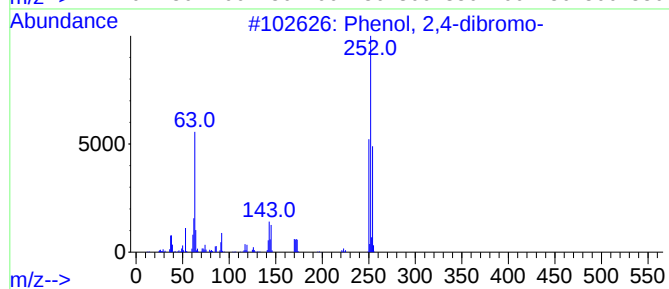
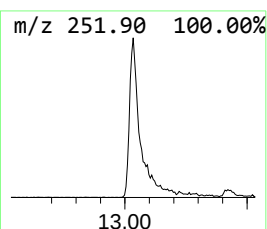
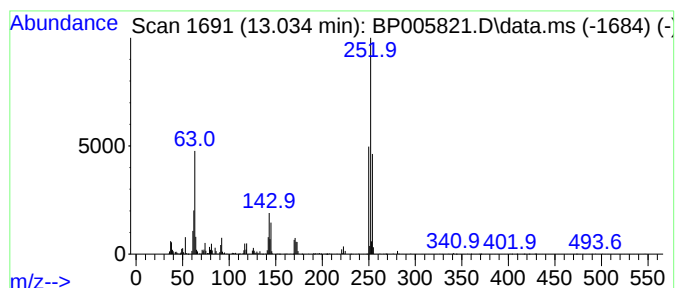
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Peak Number 3 Phenol, 2,4-dibromo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.034	6.56 ng	201964	Acenaphthene-d10	14.575

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	99
2			Phenol, 2,6-dibromo-	250	C6H4Br2O	000608-33-3	97
3			2-Pyridinamine, 3,5-dibromo-	250	C5H4Br2N2	035486-42-1	47
4			Benzene, 1,2,3,5-tetrachloro-4,6...	250	C6Cl4F2	001198-56-7	12
5			Mercury, chloromethyl-	252	CH3ClHg	000115-09-3	12



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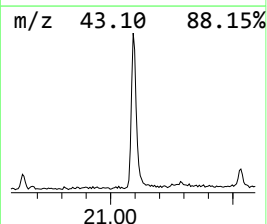
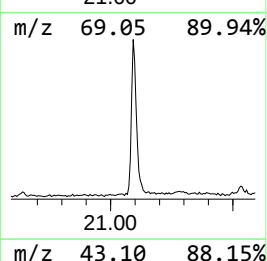
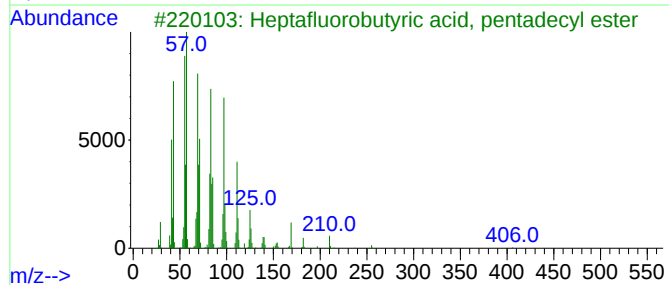
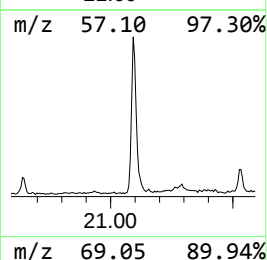
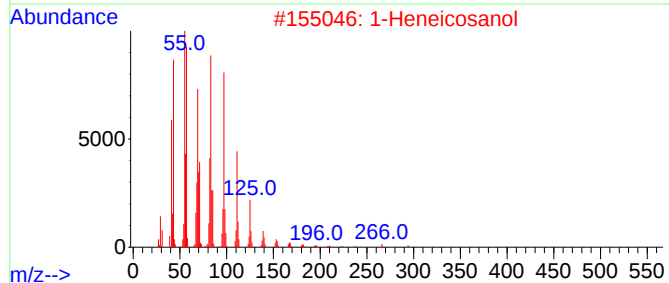
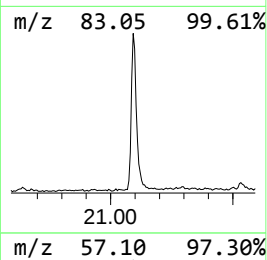
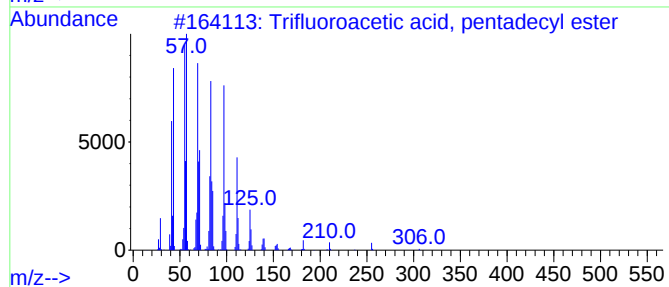
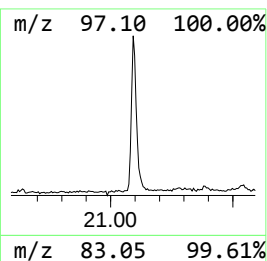
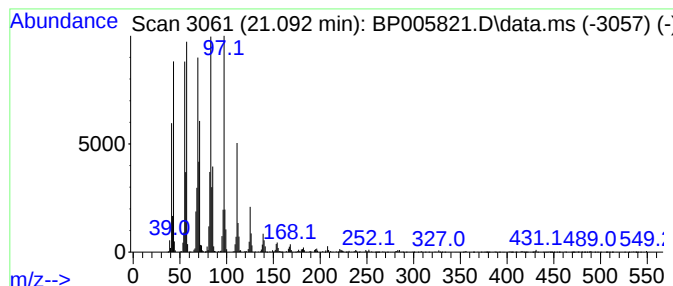
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Peak Number 4 Trifluoroacetic acid, penta... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	10.10 ng	540339	Chrysene-d12	21.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5			Behenic alcohol	326	C22H46O	000661-19-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.122	3.122	2.8	ng	52401	1	7.952	370617	20.0
2-Pentanone, 4-...	5.052	4.8	ng	87948	1	7.952	370617	20.0
Phenol, 2,4-dib...	13.034	6.6	ng	201964	3	14.575	615857	20.0
Trifluoroacetic...	21.092	10.1	ng	540339	5	21.386	1070270	20.0