

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010521\
 Data File : BG047872.D
 Acq On : 5 Jan 2021 18:16
 Operator : CG/JU
 Sample : M1007-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 R-LA-22-1-WC

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-BG121720.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047872.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.253	320	326	333	rVB3	21421	37320	2.20%	0.421%
2	5.728	400	407	414	rBV	412556	669617	39.44%	7.552%
3	7.338	673	681	692	rBV	443859	748659	44.09%	8.443%
4	7.767	748	754	759	rBV	11712	21404	1.26%	0.241%
5	8.196	819	827	835	rBV	126529	216239	12.73%	2.439%
6	9.365	1016	1026	1034	rVB	277648	491202	28.93%	5.540%
7	11.022	1301	1308	1316	rVB	152821	268508	15.81%	3.028%
8	13.443	1713	1720	1727	rBV	646743	999420	58.86%	11.271%
9	14.254	1852	1858	1865	rBV	129797	192090	11.31%	2.166%
10	14.818	1947	1954	1961	rBV2	241308	377161	22.21%	4.254%
11	16.157	2178	2182	2191	rBV2	106010	144824	8.53%	1.633%
12	16.298	2200	2206	2219	rBV	637940	953350	56.15%	10.752%
13	17.556	2414	2420	2427	rBV	324948	485530	28.59%	5.476%
14	19.777	2794	2798	2803	rVB6	24054	29250	1.72%	0.330%
15	20.141	2854	2860	2867	rVB	1317783	1697991	100.00%	19.150%
16	20.781	2963	2969	2972	rBV5	50606	71663	4.22%	0.808%
17	20.817	2972	2975	2980	rVB7	20706	31168	1.84%	0.352%
18	21.122	3019	3027	3028	rBV7	7817	17860	1.05%	0.201%
19	21.439	3075	3081	3090	rBV5	83698	185661	10.93%	2.094%
20	21.528	3092	3096	3101	rVB	17795	29617	1.74%	0.334%
21	21.827	3141	3147	3154	rBV	335718	575685	33.90%	6.493%
22	24.177	3541	3547	3549	rBV6	12821	21673	1.28%	0.244%
23	25.176	3706	3717	3727	rVB3	205868	601023	35.40%	6.778%

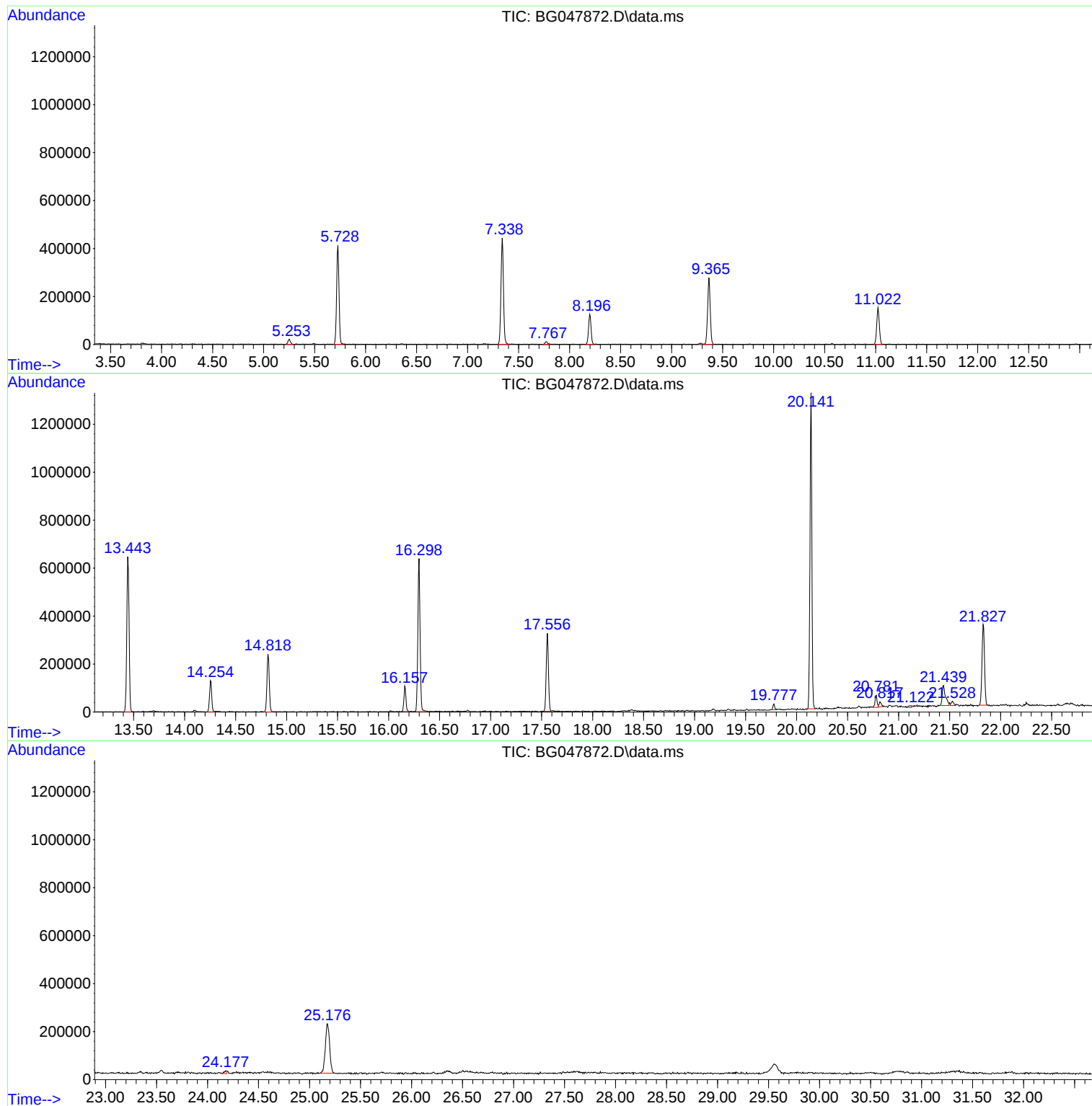
Sum of corrected areas: 8866915

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



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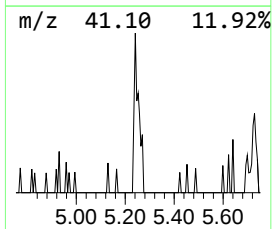
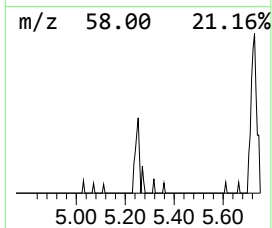
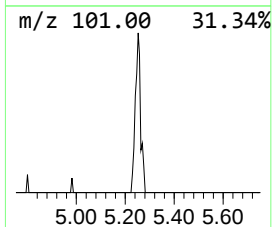
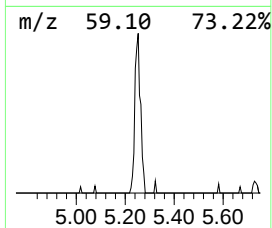
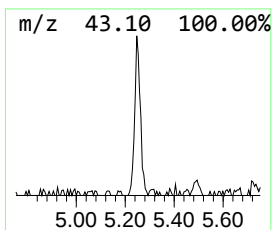
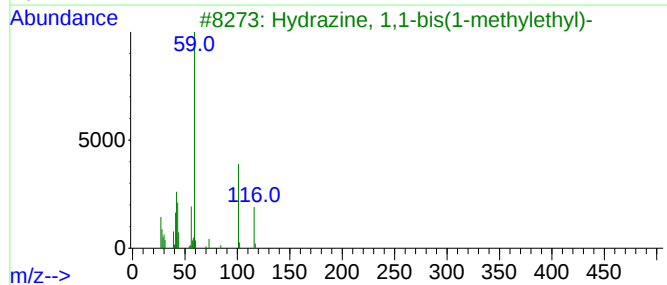
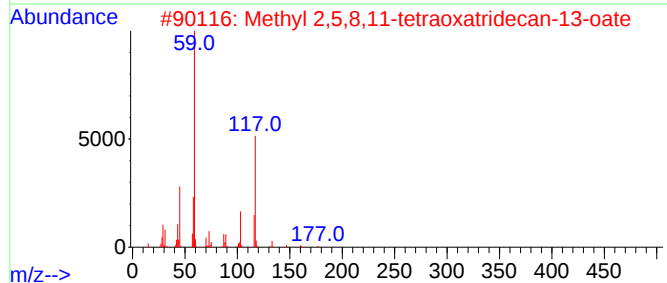
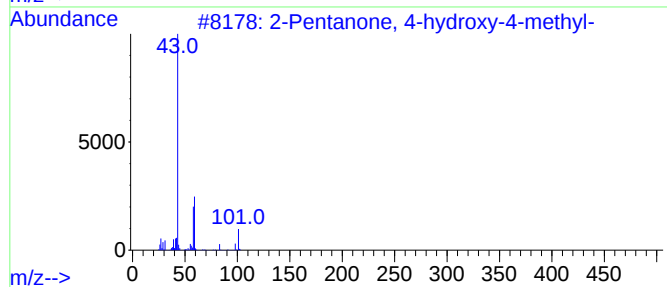
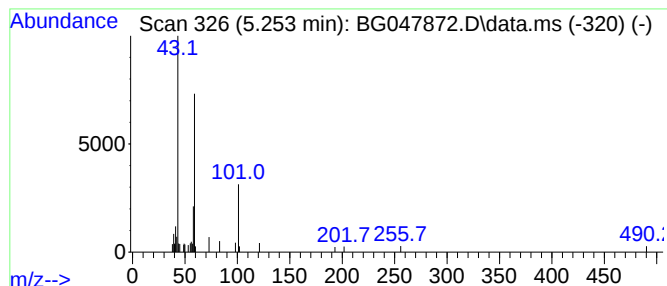
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.253	3.45 ng	37320	1,4-Dichlorobenzene-d4	8.196

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	40		
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	40		
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	38		
5	(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	36		



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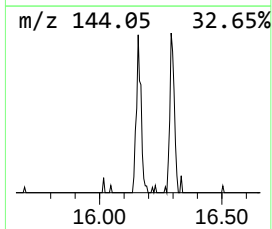
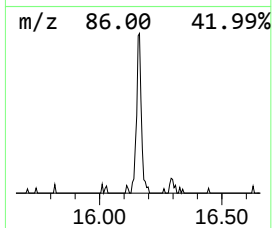
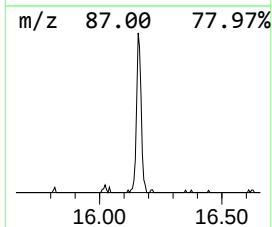
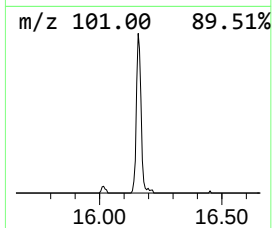
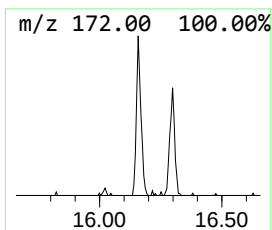
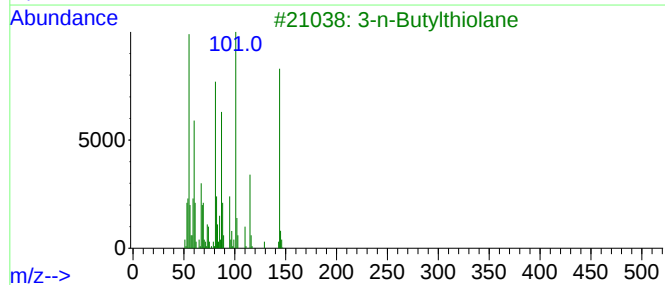
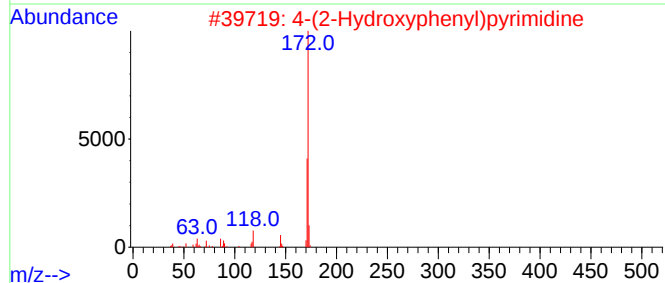
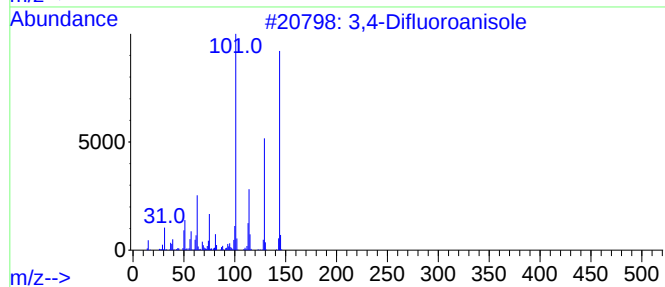
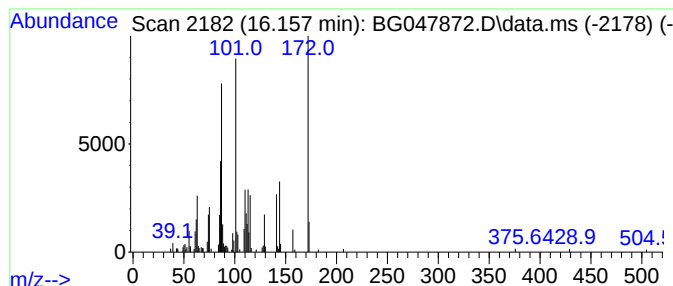
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Peak Number 2 unknown16.157 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.157	7.68 ng	144824	Acenaphthene-d10	14.818

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,4-Difluoroanisole	144	C7H6F2O	115144-40-6	30
2			4-(2-Hydroxyphenyl)pyrimidine	172	C10H8N2O	068535-55-7	10
3			3-n-Butylthiolane	144	C8H16S	001551-24-2	10
4			5-(4-Hydroxyphenyl)pyrimidine	172	C10H8N2O	069491-51-6	10
5			Succinic acid, di(3-hexyl) ester	286	C16H30O4	1000349-46-0	10



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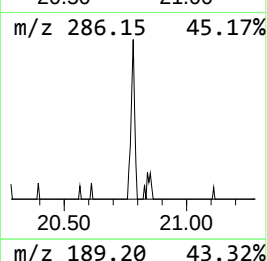
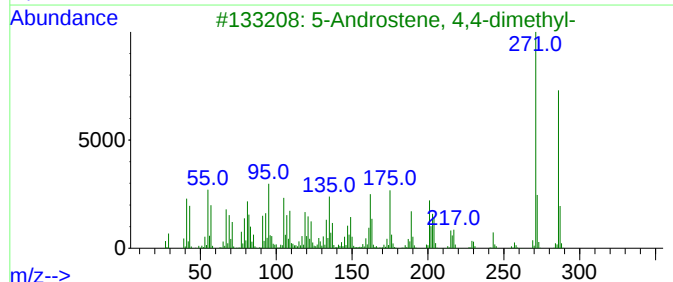
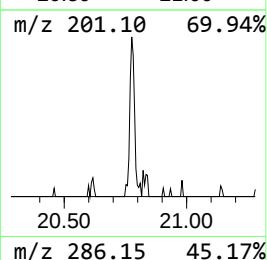
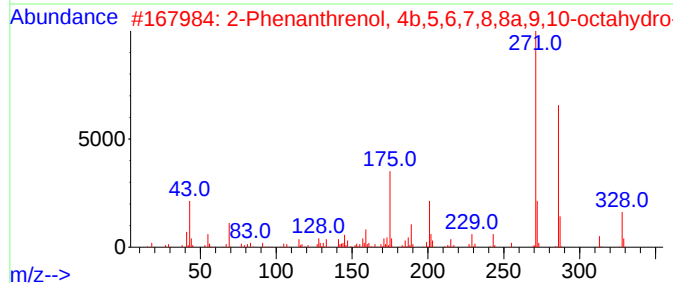
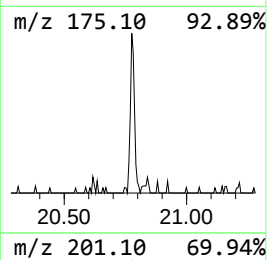
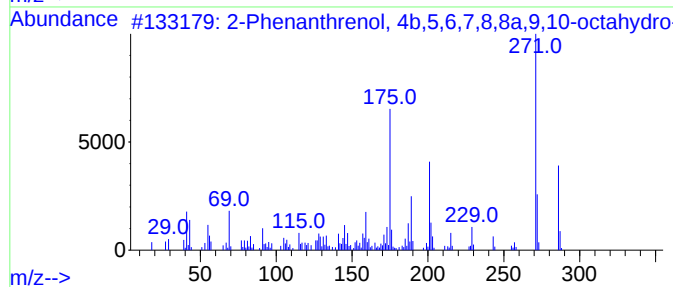
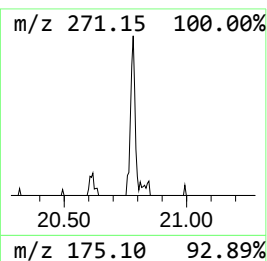
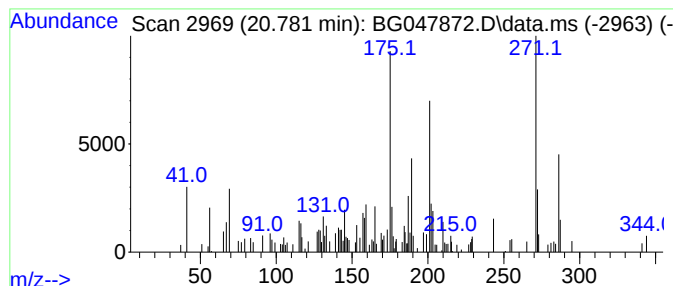
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Peak Number 3 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.781	2.49 ng	71663	Chrysene-d12	21.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	81		
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	64		
3	5-Androstene, 4,4-dimethyl-	286	C21H34	1000194-15-4	64		
4	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	46		
5	Silane, dimethyl(2-chlorophenoxy...	286	C14H23ClO2Si	1000347-07-2	38		



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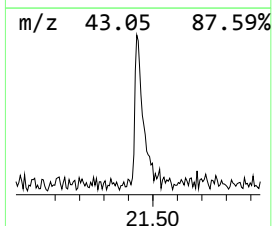
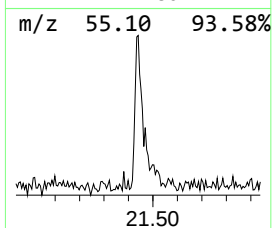
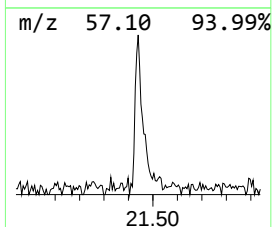
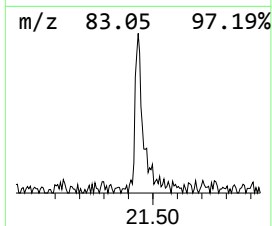
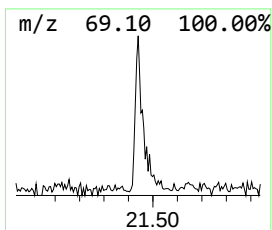
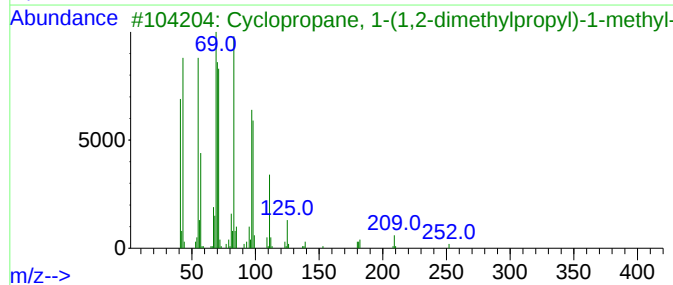
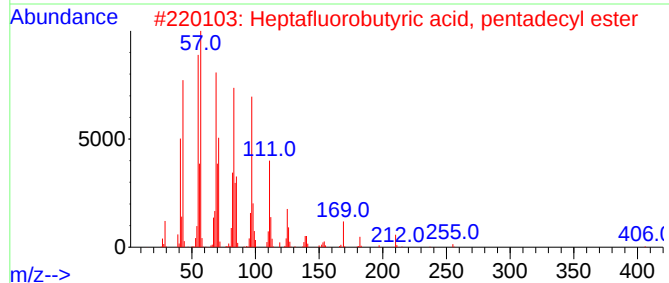
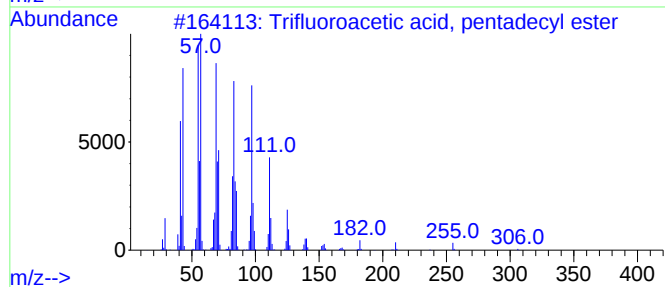
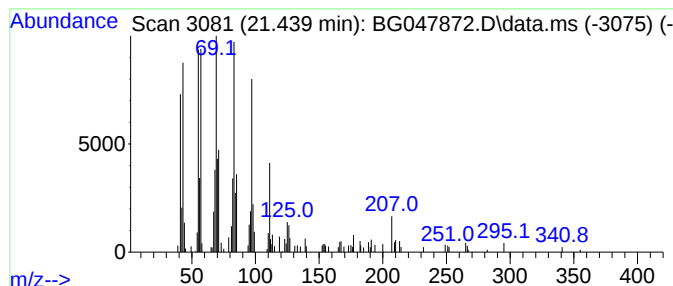
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Peak Number 4 Trifluoroacetic acid, penta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.439	6.45 ng	185661	Chrysene-d12	21.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	86
4			4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	86
5			Cyclohexadecane	224	C16H32	000295-65-8	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.253	3.5	ng	37320	1	8.196	216239	20.0
unknown16.157	16.157	7.7	ng	144824	3	14.818	377161	20.0
2-Phenanthrenol...	20.781	2.5	ng	71663	5	21.827	575685	20.0
Trifluoroacetic...	21.439	6.5	ng	185661	5	21.827	575685	20.0