

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
 Data File : BM016355.D
 Acq On : 14 Aug 2018 15:24
 Operator : SJ/JU
 Sample : J4442-11
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-1-2

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_M\METHODS\8270-BM072318.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.169	314	320	332	rBV	111547	171436	7.86%	1.251%
2	5.646	396	401	419	rBV	768520	1159533	53.17%	8.463%
3	7.287	674	680	693	rBV	787119	1240626	56.89%	9.054%
4	7.645	735	741	757	rBB	861081	1352486	62.02%	9.871%
5	8.116	815	821	830	rBB	173841	279138	12.80%	2.037%
6	8.434	869	875	884	rBV	612242	996360	45.69%	7.272%
7	9.304	1016	1023	1038	rBV	453841	756790	34.70%	5.523%
8	10.928	1293	1299	1310	rBV	197879	337481	15.48%	2.463%
9	13.369	1708	1714	1725	rBV	1083336	1536083	70.44%	11.211%
10	14.204	1852	1856	1864	rVB	61318	84671	3.88%	0.618%
11	14.751	1944	1949	1957	rVB3	277661	409709	18.79%	2.990%
12	16.239	2197	2202	2214	rBV	1110716	1528214	70.08%	11.153%
13	17.486	2409	2414	2424	rVB2	326091	473877	21.73%	3.458%
14	18.339	2554	2559	2566	rBV	90145	117985	5.41%	0.861%
15	19.598	2769	2773	2779	rBV3	30774	39917	1.83%	0.291%
16	20.068	2848	2853	2858	rBV	1856190	2180637	100.00%	15.915%
17	21.292	3057	3061	3067	rBV4	64443	109490	5.02%	0.799%
18	21.621	3112	3117	3123	rBV	370973	470641	21.58%	3.435%
19	23.950	3507	3513	3523	rVB	238615	456804	20.95%	3.334%

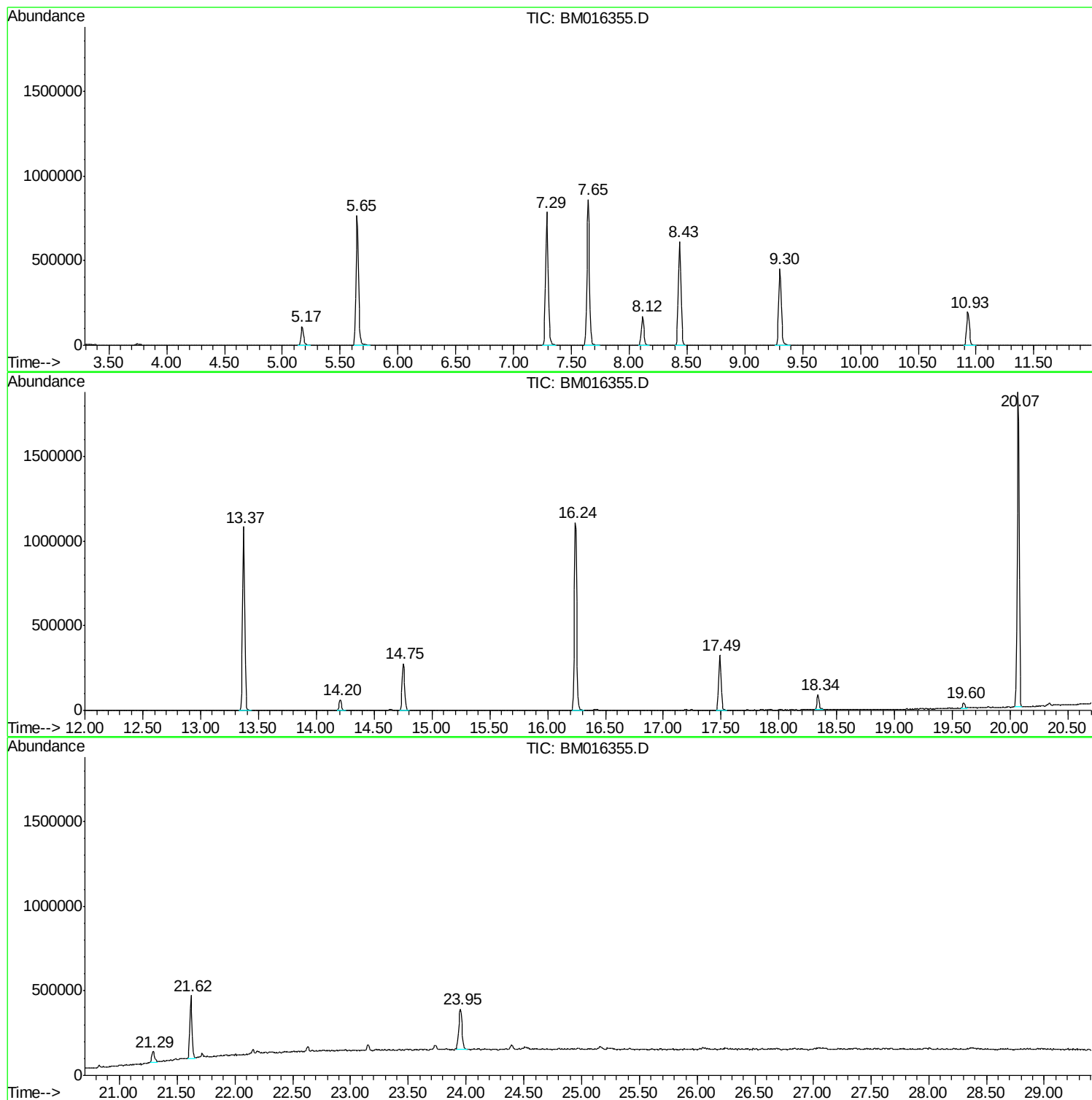
Sum of corrected areas: 13701878

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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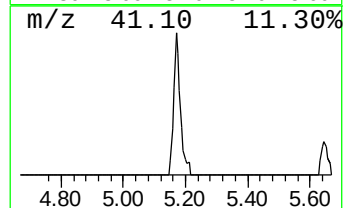
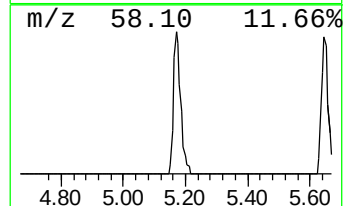
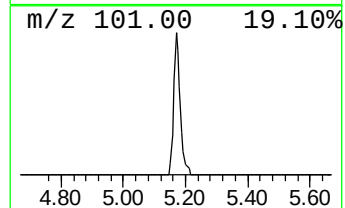
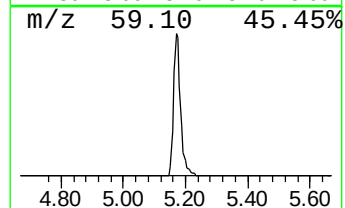
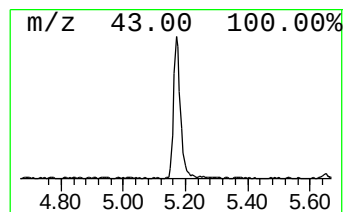
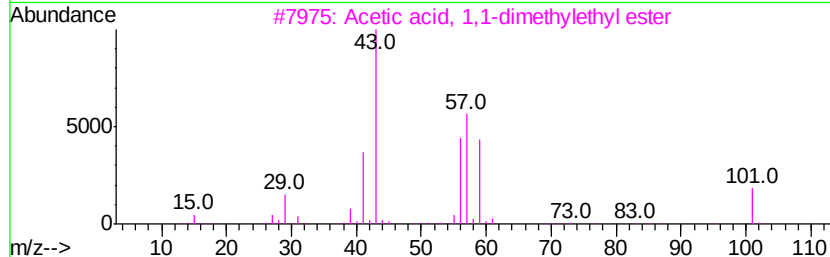
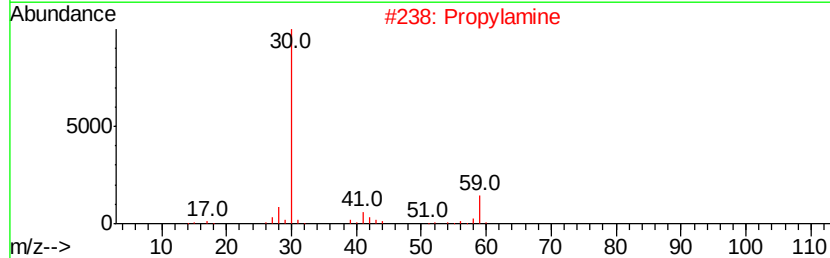
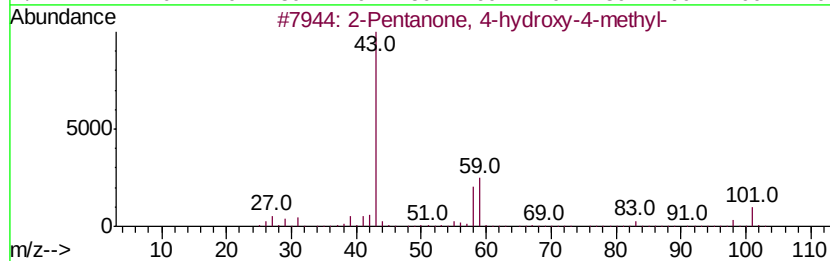
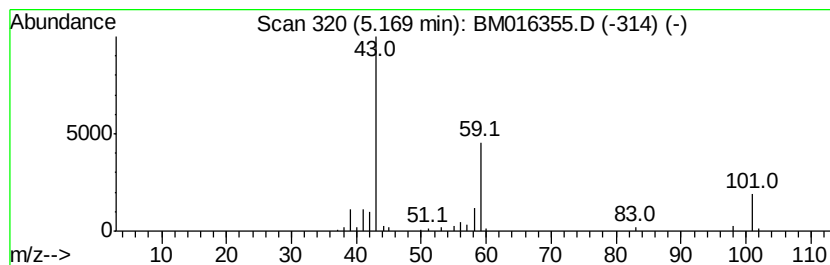
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	12.28 ng	171436	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Propylamine	59	C3H9N	000107-10-8	38
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
5			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33



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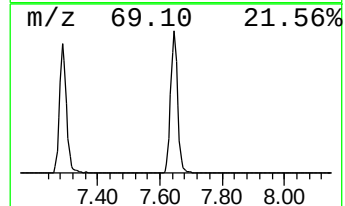
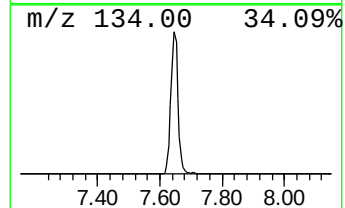
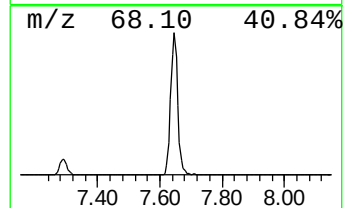
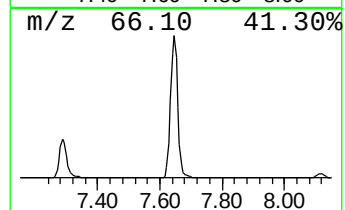
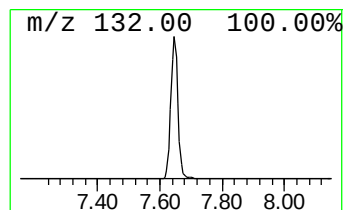
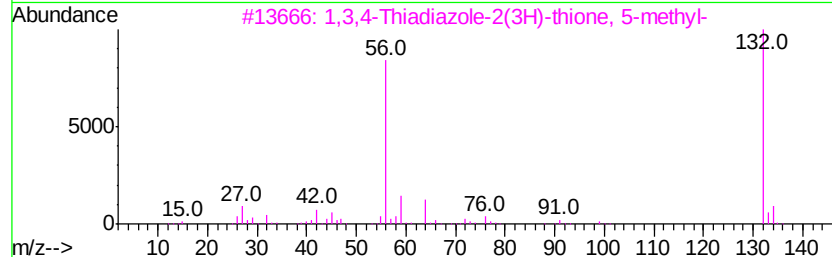
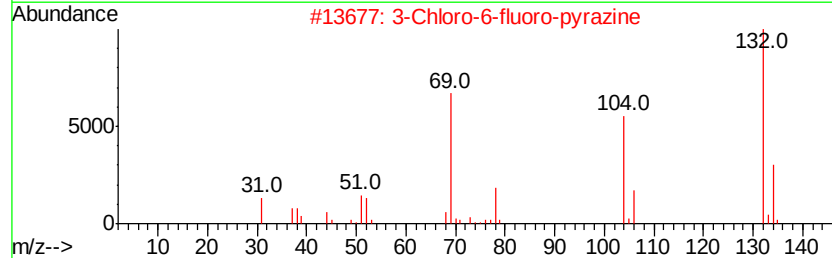
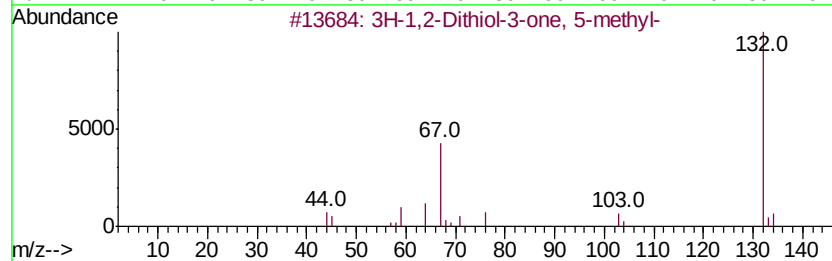
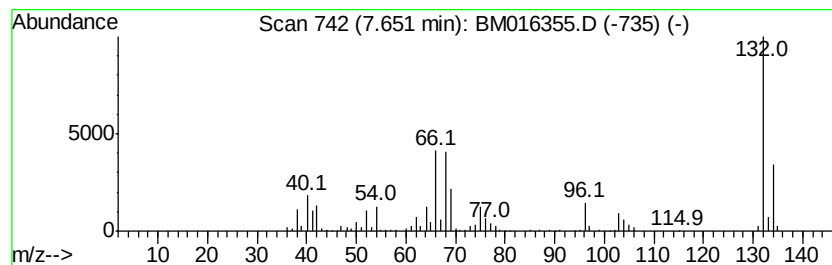
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Peak Number 2 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	96.90 ng	1352490	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	10



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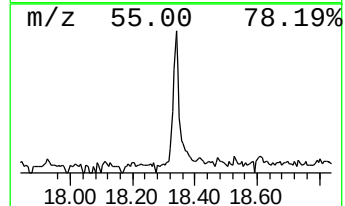
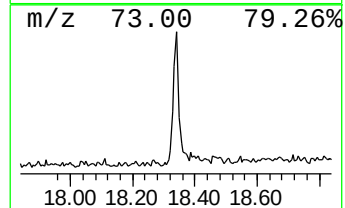
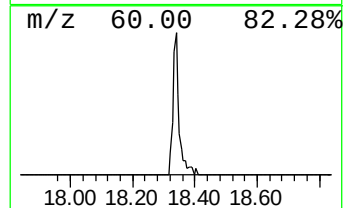
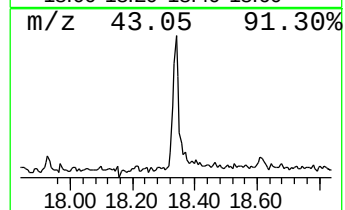
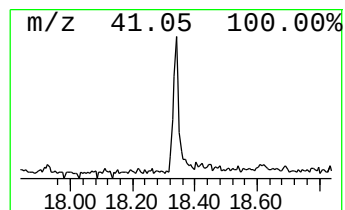
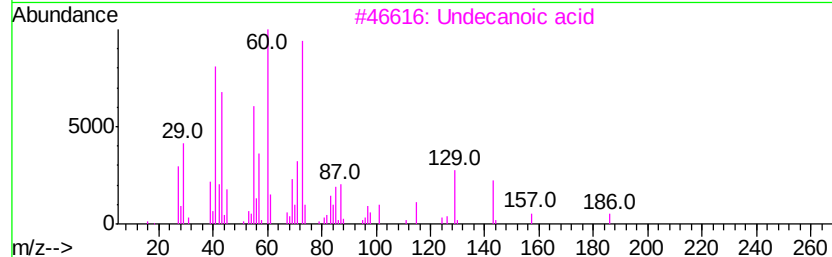
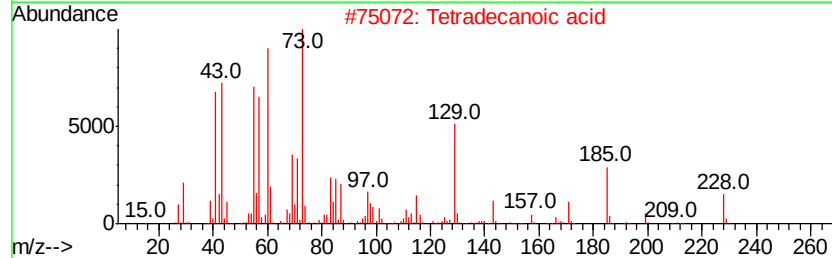
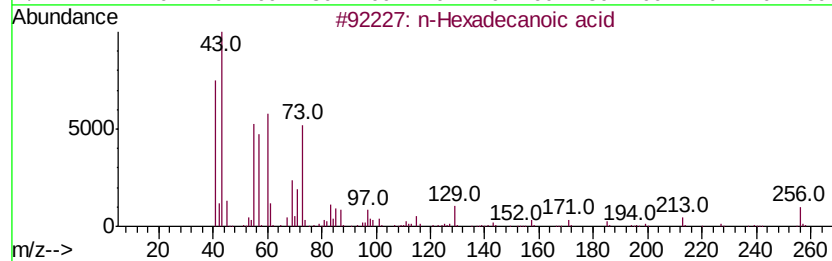
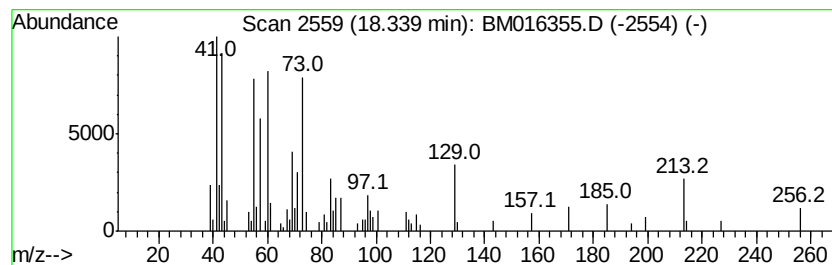
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.34	4.98 ng	117985	Phenanthrene-d10		17.49
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3	Undecanoic acid	186	C11H22O2	000112-37-8	52
4	n-Decanoic acid	172	C10H20O2	000334-48-5	47
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47



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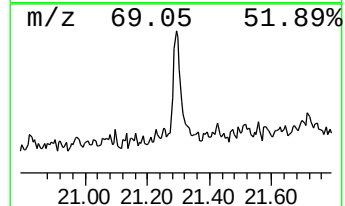
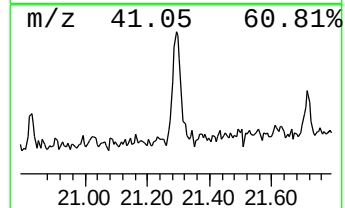
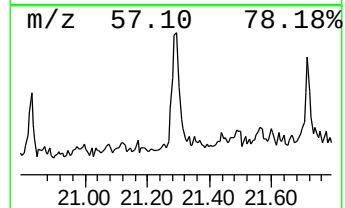
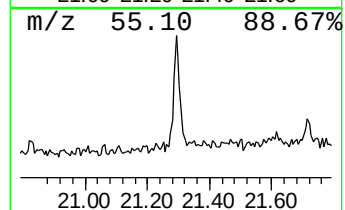
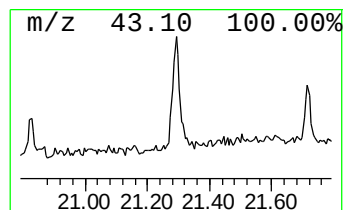
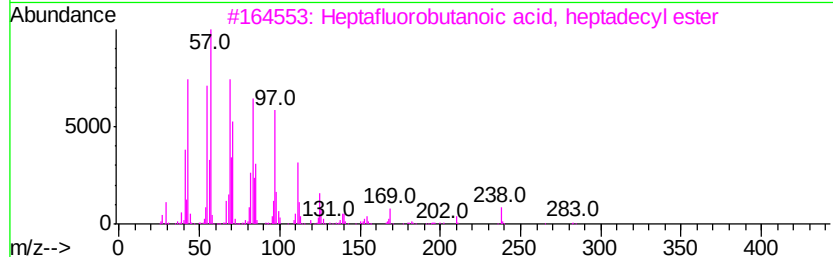
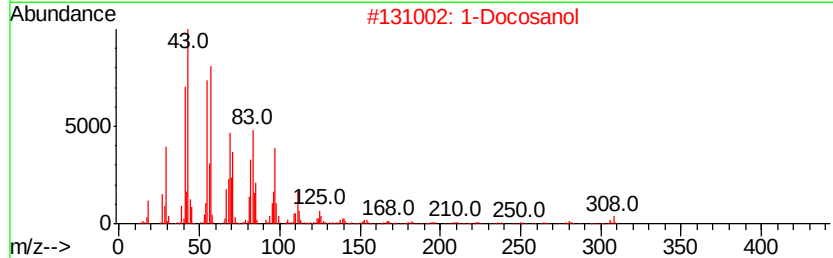
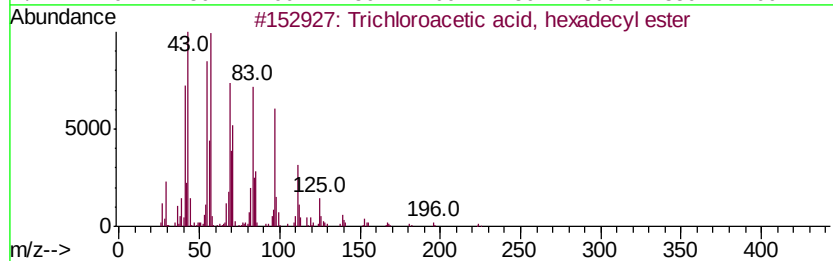
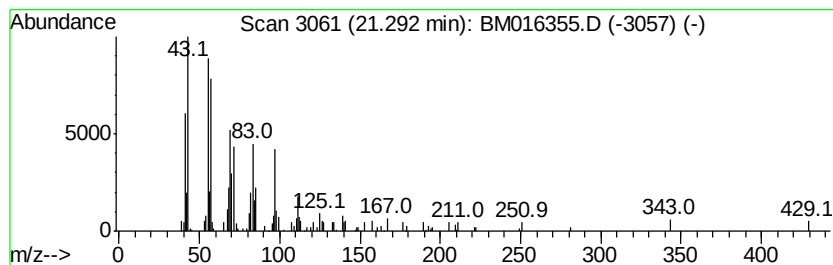
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Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	4.65 ng	109490	Chrysene-d12	21.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2		1-Docosanol	326	C22H46O	000661-19-8	90
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	90
4		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	12.3	ng	171436	1	8.12	279138	20.0
unknown7.65	7.65	96.9	ng	1352490	1	8.12	279138	20.0
n-Hexadecanoic acid	18.34	5.0	ng	117985	4	17.49	473877	20.0
Trichloroacetic a...	21.29	4.7	ng	109490	5	21.62	470641	20.0