

Data Path : Z:\HPCHEM1\BNA G\DATA\BG032718\
 Data File : BG033370.D
 Acq On : 27 Mar 2018 20:13
 Operator : SJ/JU
 Sample : J2038-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 032218-TIDO-F-D-S

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:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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	3.479	26	32	43	rBV2	114072	246257	5.81%	1.519%
2	3.573	43	48	59	rVB2	89694	148958	3.52%	0.919%
3	6.288	504	510	530	rBV2	137298	326794	7.71%	2.016%
4	7.974	788	797	809	rBV	79124	215357	5.08%	1.329%
5	8.379	856	866	880	rBV	312227	691594	16.33%	4.267%
6	8.867	942	949	969	rBV2	100655	255149	6.02%	1.574%
7	9.202	995	1006	1021	rBV	529741	1081050	25.52%	6.669%
8	10.065	1145	1153	1170	rBV	421946	969678	22.89%	5.982%
9	11.752	1431	1440	1451	rBV	162506	348513	8.23%	2.150%
10	14.114	1835	1842	1856	rBV	1499935	2581017	60.93%	15.923%
11	14.901	1969	1976	1987	rBV	31338	52742	1.24%	0.325%
12	15.483	2069	2075	2089	rBV2	335932	580739	13.71%	3.583%
13	16.252	2200	2206	2210	rBV	33571	45165	1.07%	0.279%
14	16.957	2319	2326	2342	rBV	828568	1475153	34.82%	9.101%
15	17.104	2346	2351	2361	rVB	37829	68498	1.62%	0.423%
16	18.215	2529	2540	2553	rBV	468344	834952	19.71%	5.151%
17	19.008	2671	2675	2685	rBV4	32600	64563	1.52%	0.398%
18	20.735	2962	2969	2982	rBV	2999317	4236314	100.00%	26.135%
19	22.075	3191	3197	3205	rBV4	46856	96526	2.28%	0.595%
20	22.557	3272	3279	3289	rBV	462233	922904	21.79%	5.694%
21	24.078	3532	3538	3547	rBV10	28834	97153	2.29%	0.599%
22	26.323	3909	3920	3933	rBV	266566	870276	20.54%	5.369%

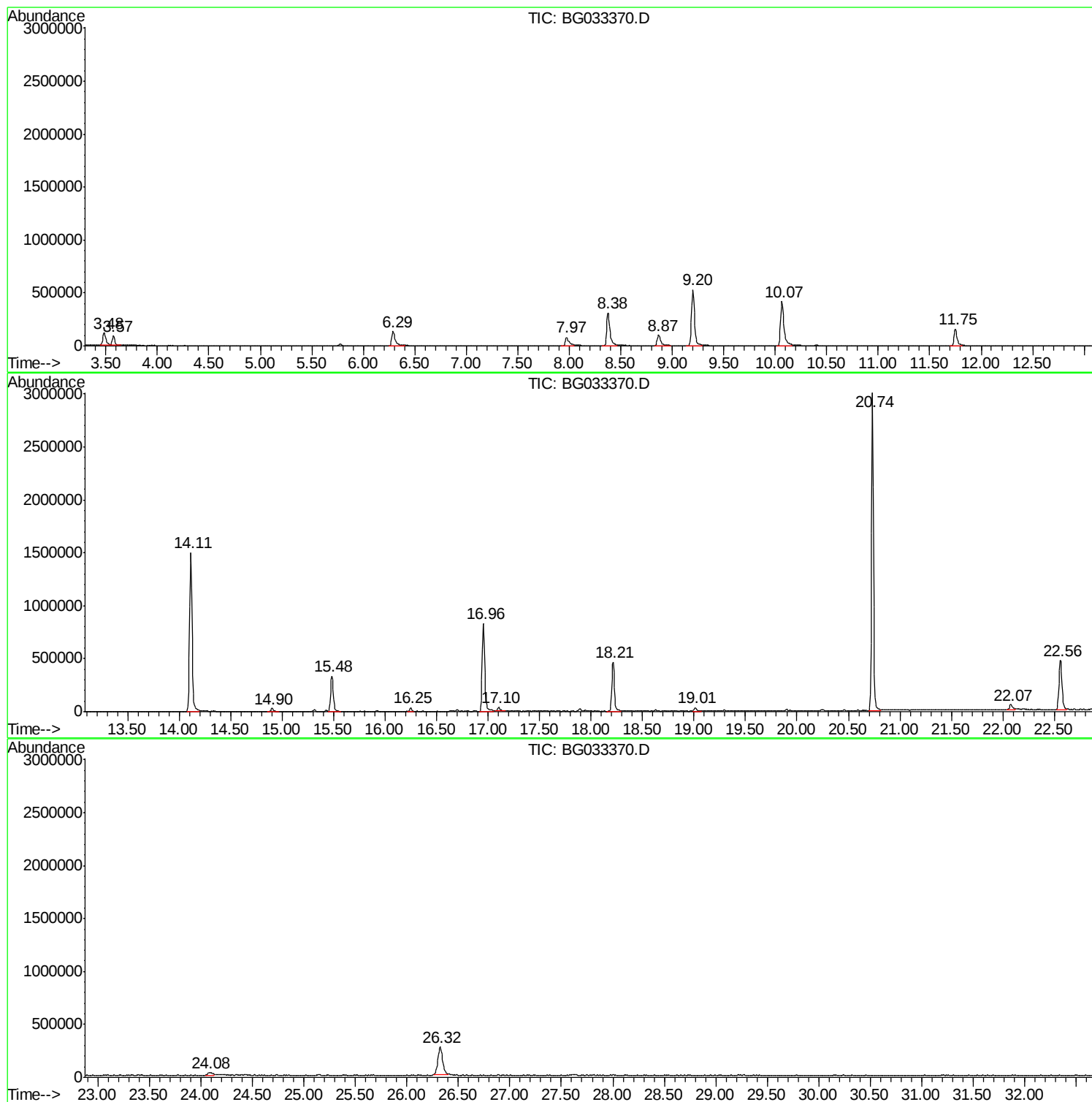
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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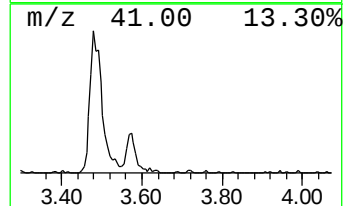
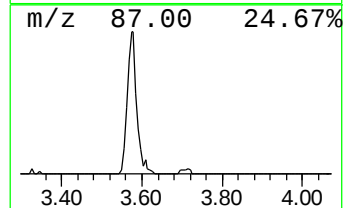
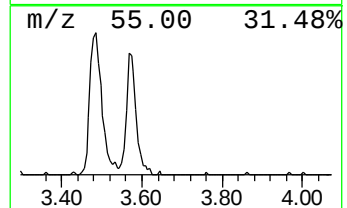
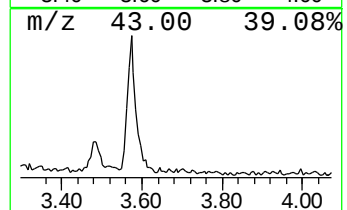
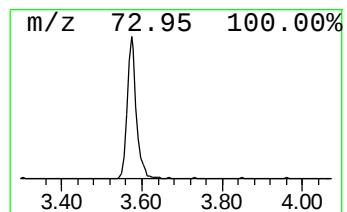
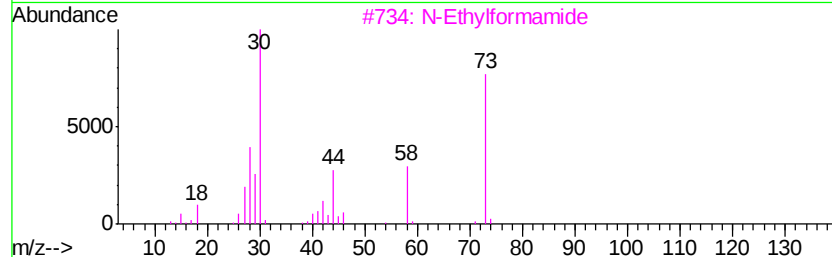
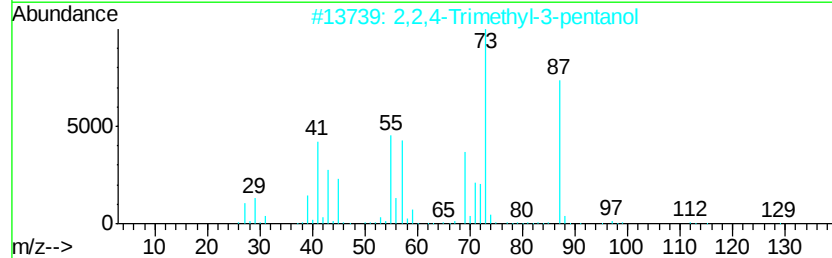
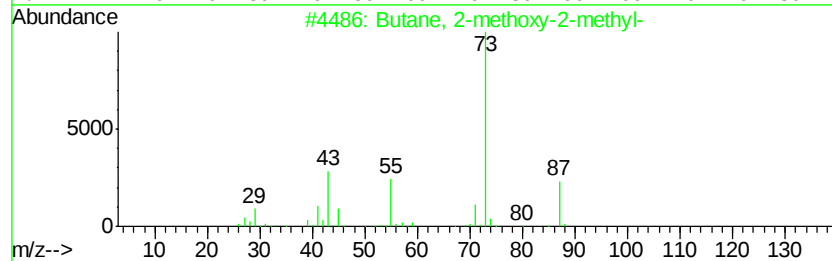
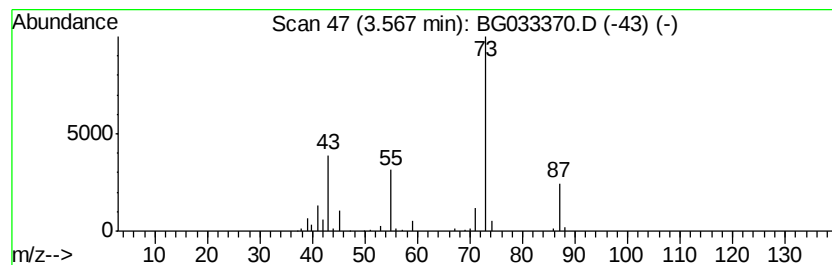
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	11.68 ng	148958	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9



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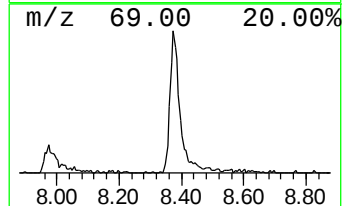
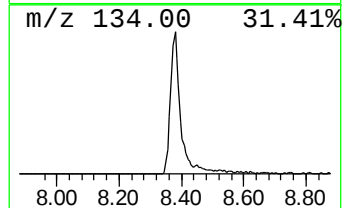
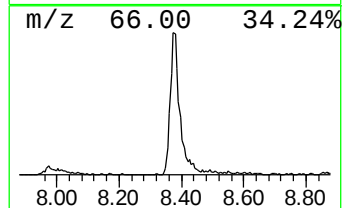
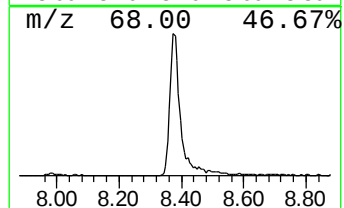
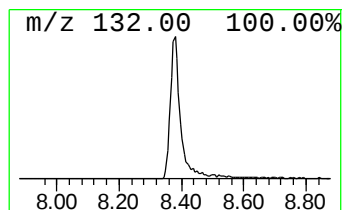
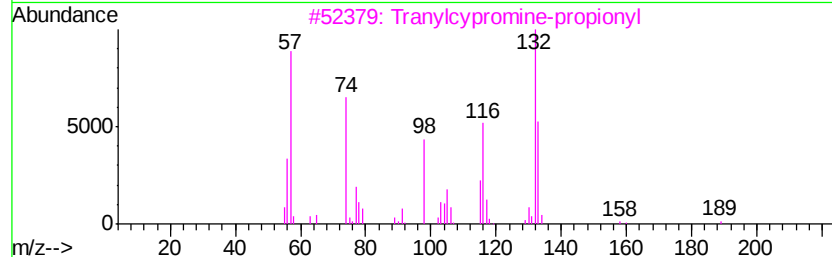
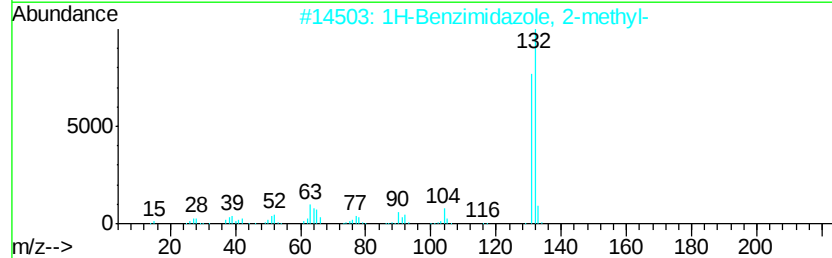
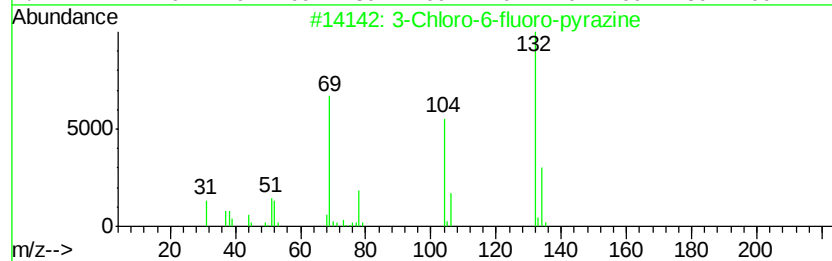
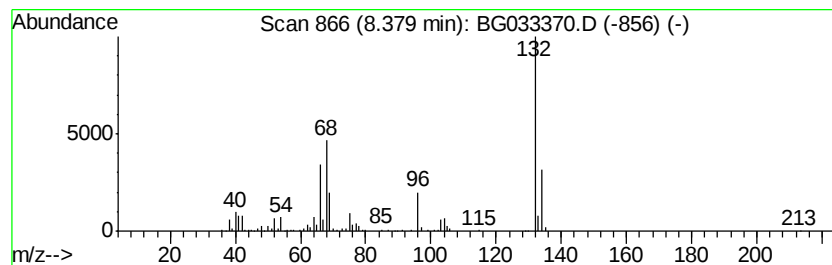
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Peak Number 3 unknown8.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	54.21 ng	691594	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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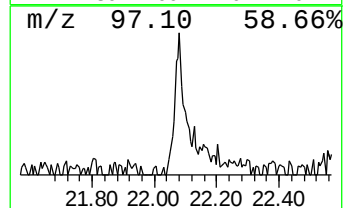
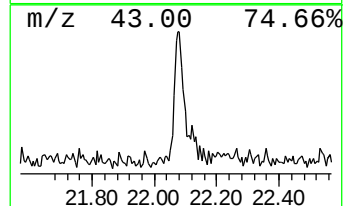
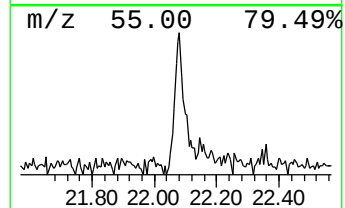
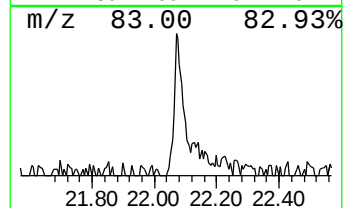
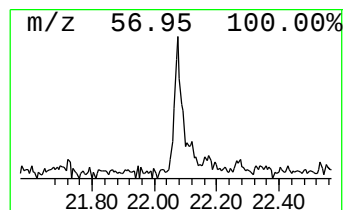
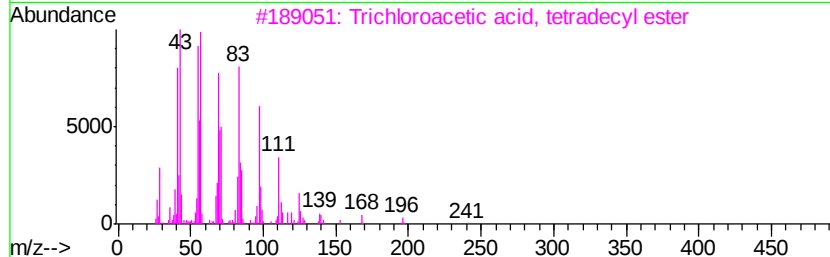
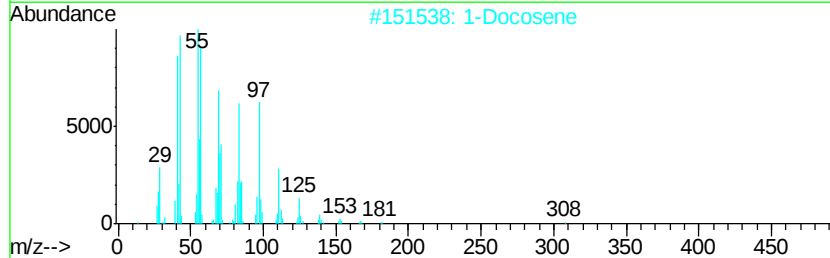
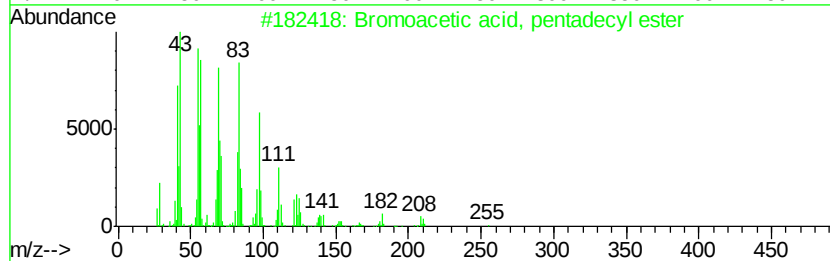
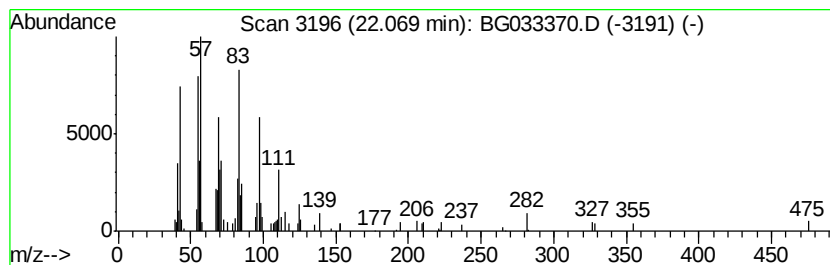
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Peak Number 5 Bromoacetic acid, pentadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	2.09 ng	96526	Chrysene-d12	22.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87
2		1-Docosene	308	C22H44	001599-67-3	83
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	83
4		Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	81
5		1,2-Octadecanediol	286	C18H38O2	020294-76-2	80



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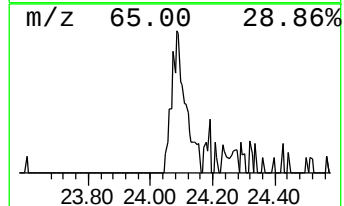
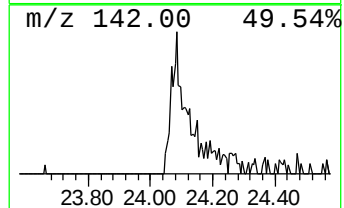
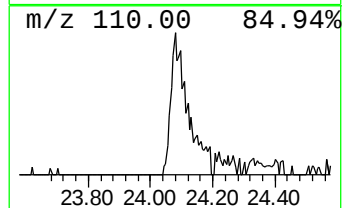
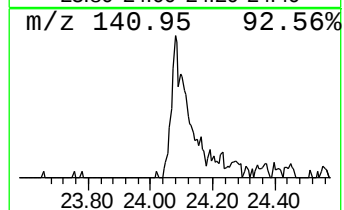
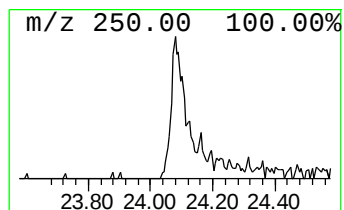
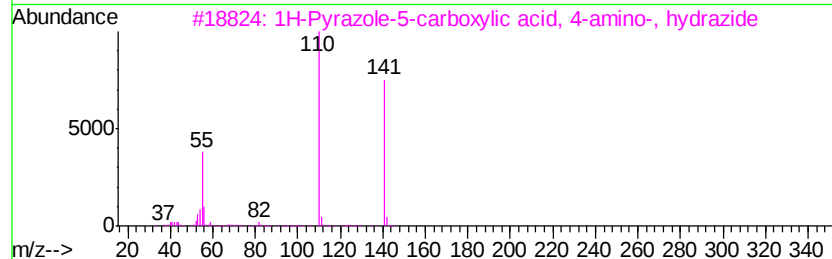
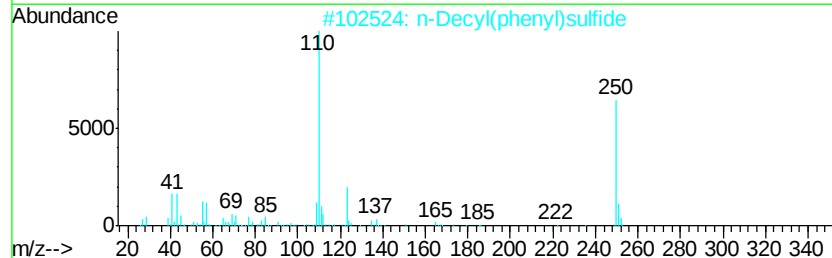
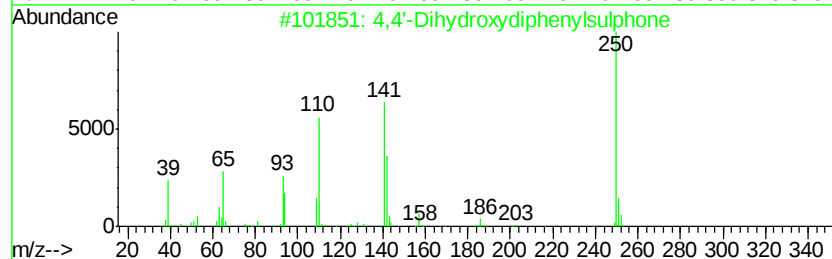
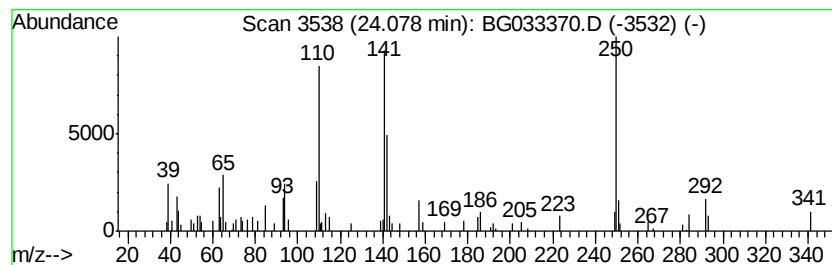
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Peak Number 6 4,4'-Dihydroxydiphenylsulphone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.08	2.11 ng	97153	Chrysene-d12	22.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	93
2		n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	38
3		1H-Pyrazole-5-carboxylic acid, 4...	141	C4H7N5O	1000327-48-2	35
4		1,3-Benzenediol, o-(2,6-difluoro...	250	C13H8F2O3	1000330-83-2	32
5		4,4'-Thiodibenzenethiol	250	C12H10S3	019362-77-7	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	11.7	ng	148958	1	8.87	255149	20.0
unknown8.38	8.38	54.2	ng	691594	1	8.87	255149	20.0
Bromoacetic acid,...	22.07	2.1	ng	96526	5	22.56	922904	20.0
4,4'-Dihydroxydip...	24.08	2.1	ng	97153	5	22.56	922904	20.0