

Data Path : Z:\HPCHEM1\BNA M\DATA\BM052217\
 Data File : BM010133.D
 Acq On : 23 May 2017 09:34
 Operator : SJ/MA
 Sample : I3240-02
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 EP2-WC8(12-16)

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_M\METHODS\8270-BM051917.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	5.075	334	338	349	rBV	645407	892736	8.27%	1.581%
2	5.540	411	417	430	rBV	3263848	4599613	42.62%	8.143%
3	7.145	683	690	704	rBV	2774407	4543708	42.10%	8.044%
4	7.498	743	750	758	rBV	3098107	4817234	44.64%	8.529%
5	7.957	822	828	834	rBV	536628	885611	8.21%	1.568%
6	8.281	874	883	893	rBV	2396166	3822036	35.42%	6.767%
7	9.145	1023	1030	1039	rBV	1653779	2699132	25.01%	4.779%
8	10.769	1299	1306	1314	rVB	625541	1034610	9.59%	1.832%
9	13.210	1712	1721	1732	rBV	4338534	6418213	59.47%	11.363%
10	14.051	1858	1864	1873	rVB	497099	674151	6.25%	1.194%
11	14.592	1949	1956	1965	rBV2	912911	1381728	12.80%	2.446%
12	16.080	2203	2209	2220	rBV	4041843	5257080	48.71%	9.307%
13	17.333	2417	2422	2433	rBV2	1214164	1738533	16.11%	3.078%
14	18.180	2561	2566	2574	rBV2	116793	180973	1.68%	0.320%
15	19.939	2859	2865	2870	rBV	8880952	10791950	100.00%	19.107%
16	21.492	3124	3129	3135	rBV	2168051	2733555	25.33%	4.840%
17	22.639	3320	3324	3332	rBV	523810	1006353	9.33%	1.782%
18	23.856	3525	3531	3540	rVB	1539451	3005805	27.85%	5.322%

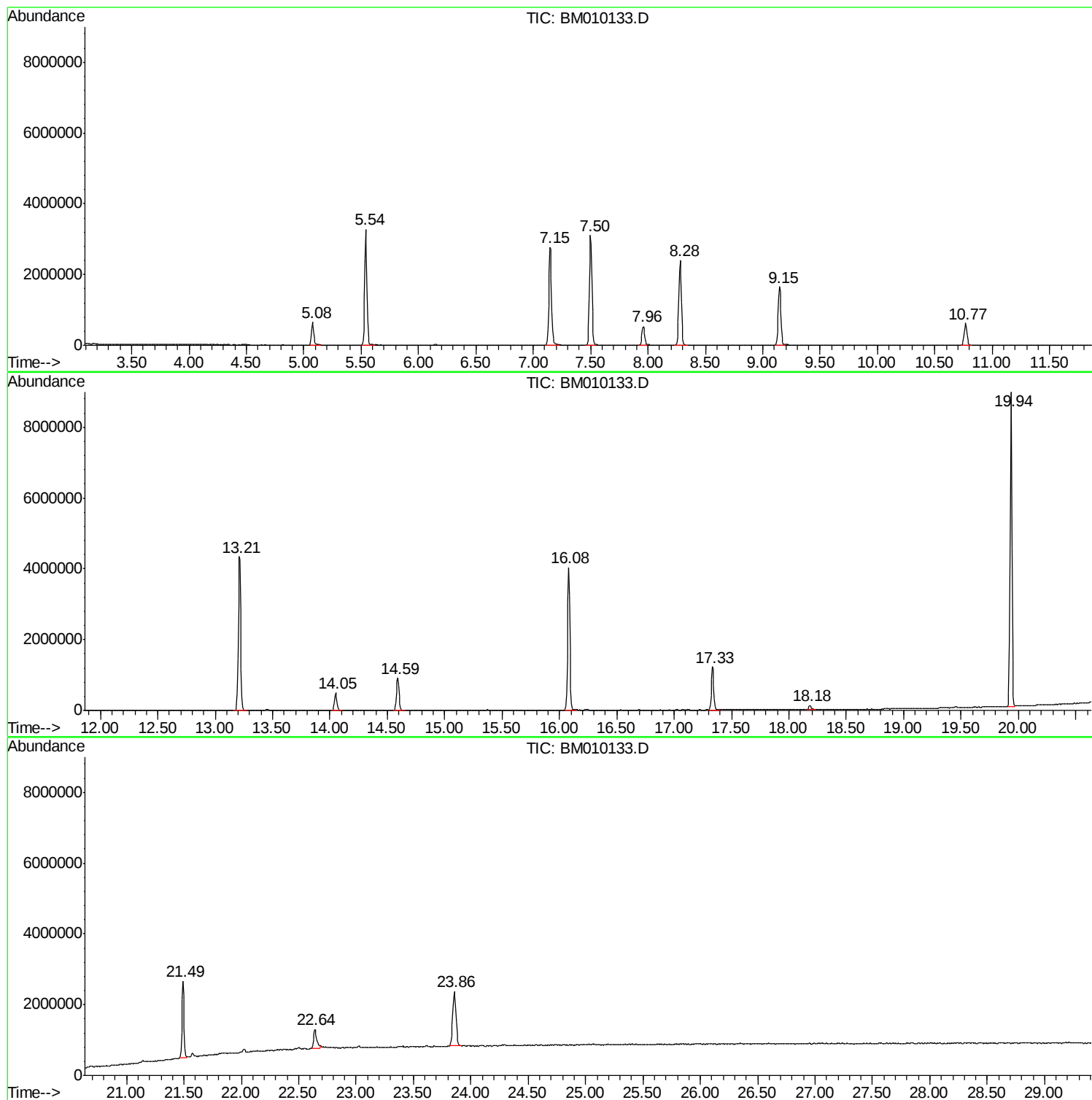
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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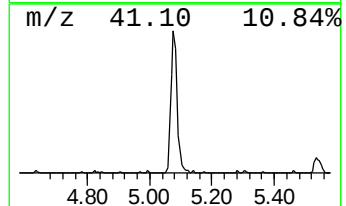
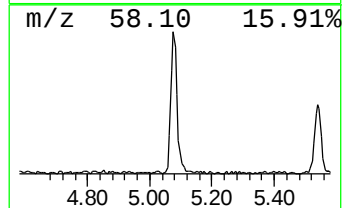
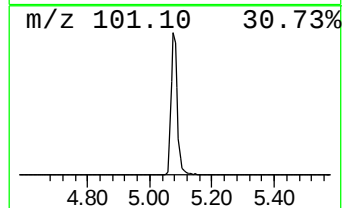
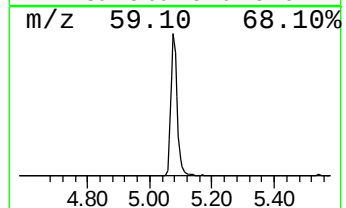
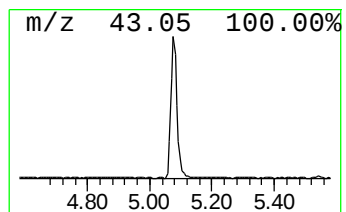
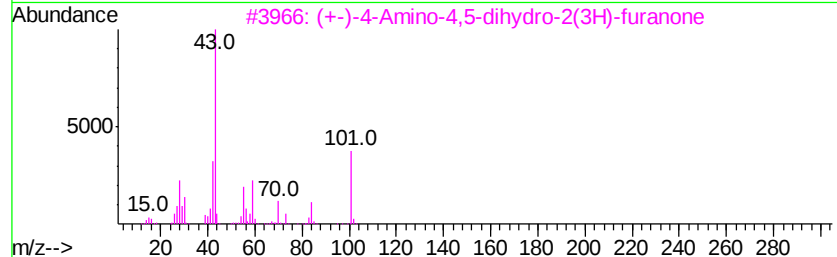
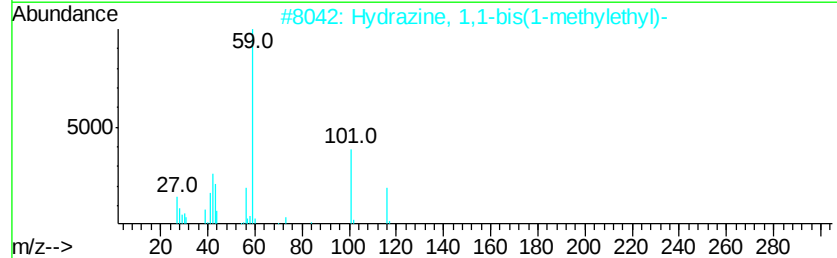
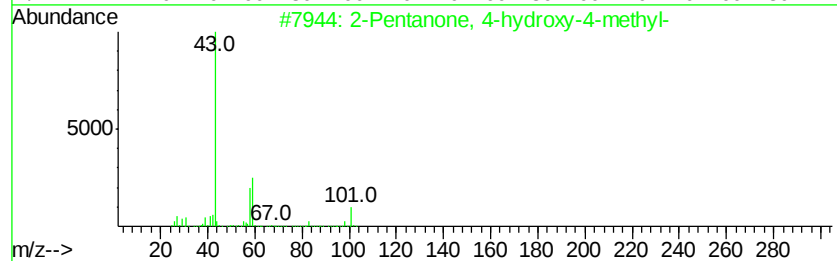
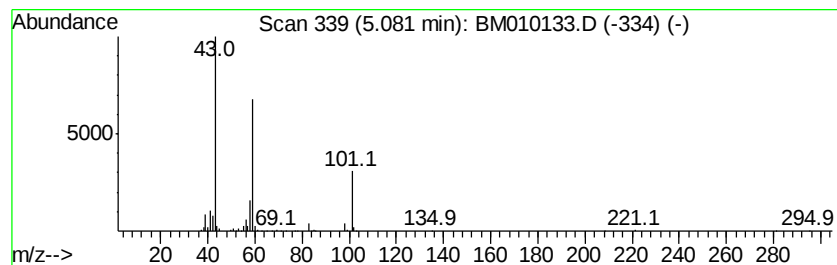
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	20.16 ng	892736	1,4-Dichlorobenzene-d4	7.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	47
3			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	38
4			Acetic acid, 10,11-dihydroxy-3,7-dimethyl-	298	C17H30O4	1000194-28-5	23
5			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17



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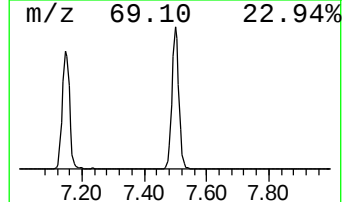
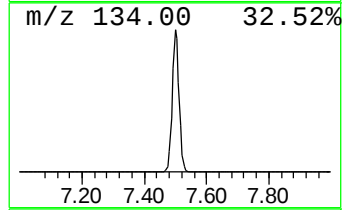
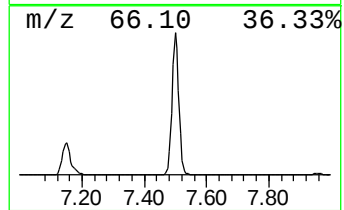
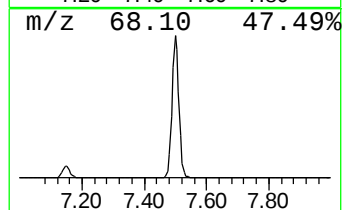
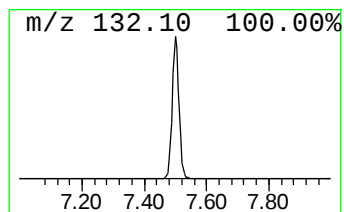
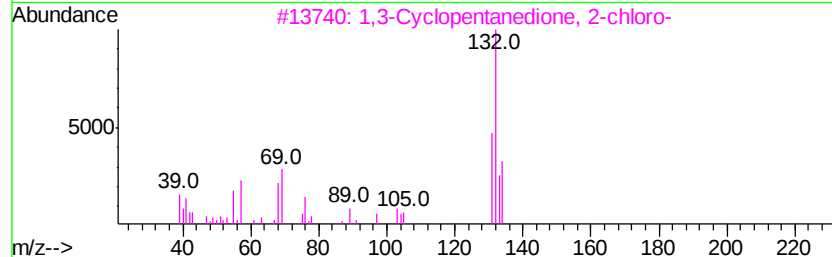
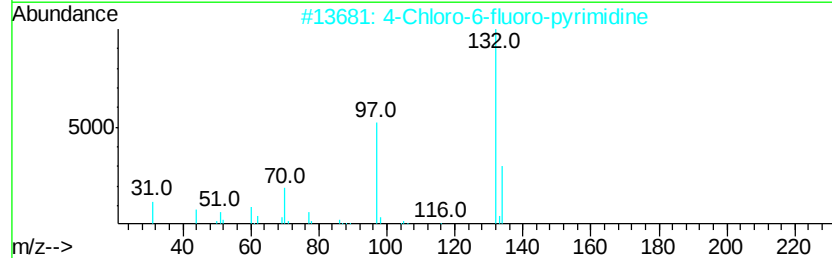
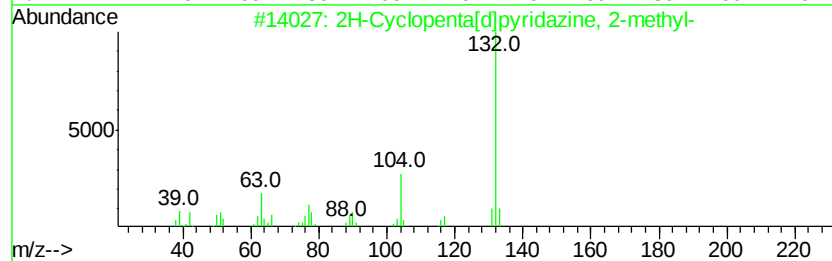
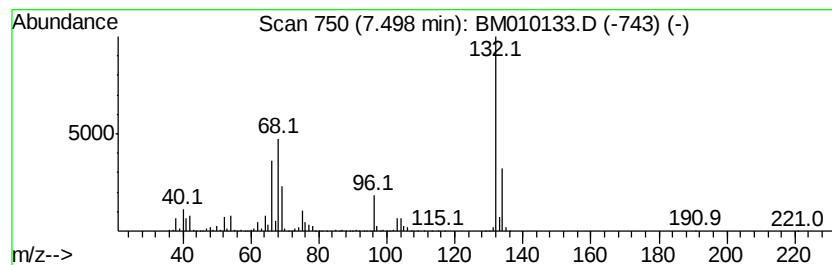
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Peak Number 2 unknown7.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.50	108.79 ng	4817230	1,4-Dichlorobenzene-d4	7.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22



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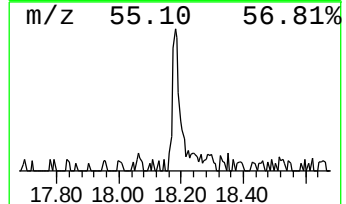
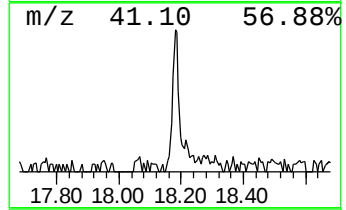
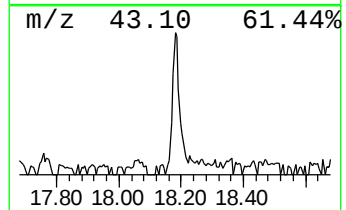
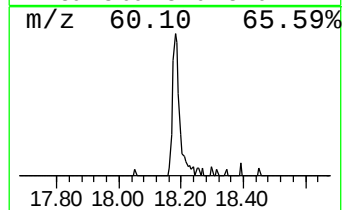
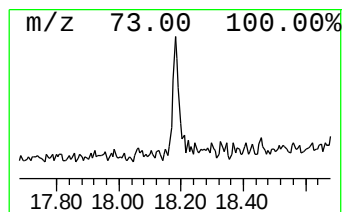
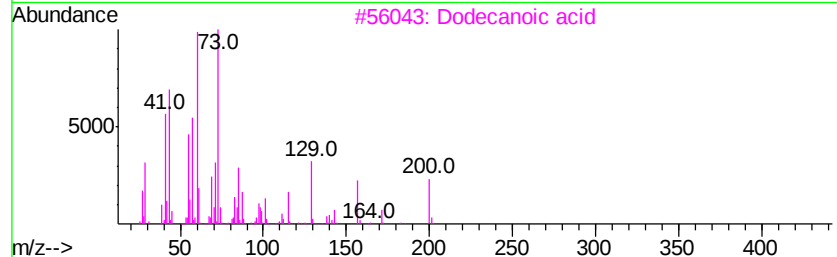
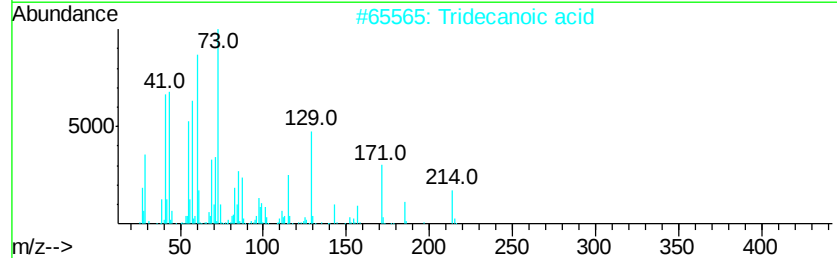
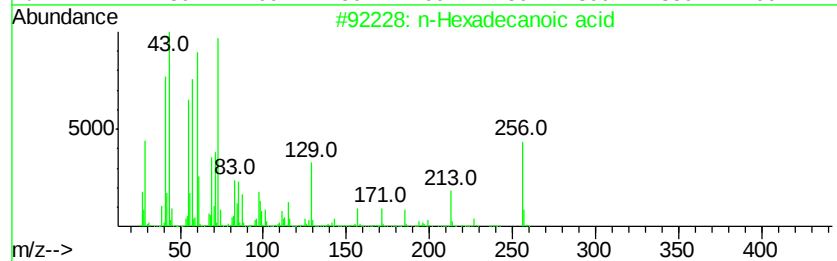
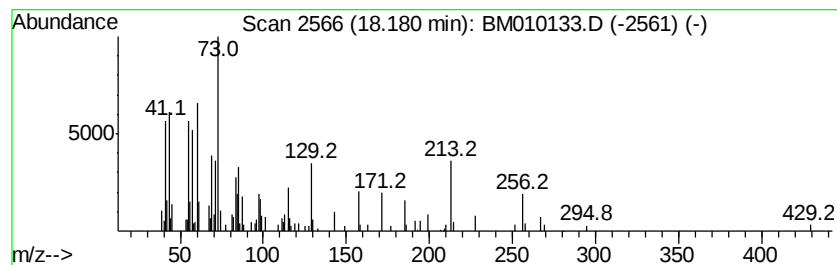
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.18	2.08 ng	180973	Phenanthrene-d10	17.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Dodecanoic acid	200	C12H24O2	000143-07-7	53
4	3,7-Dimethyl-8-oxo-1,5-dioxaspi...	256	C13H20O5	1000193-79-8	47
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	47



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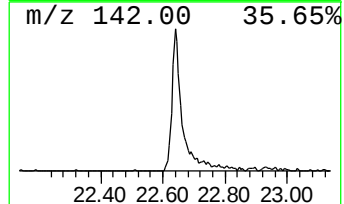
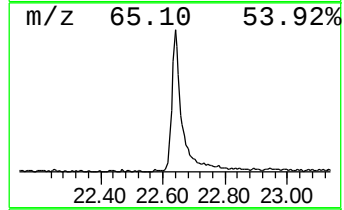
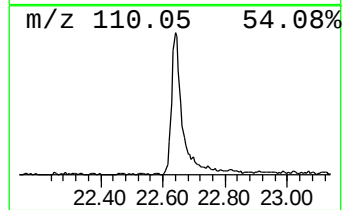
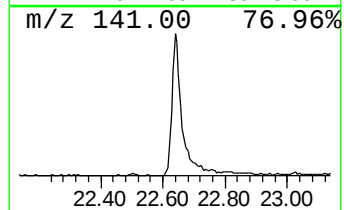
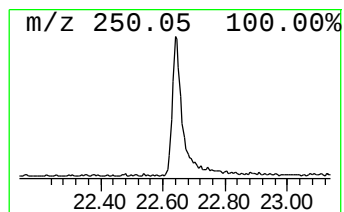
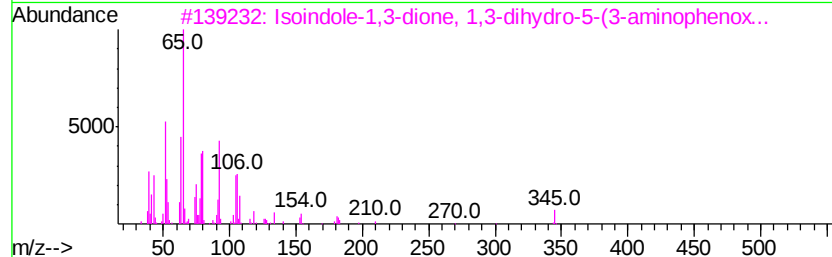
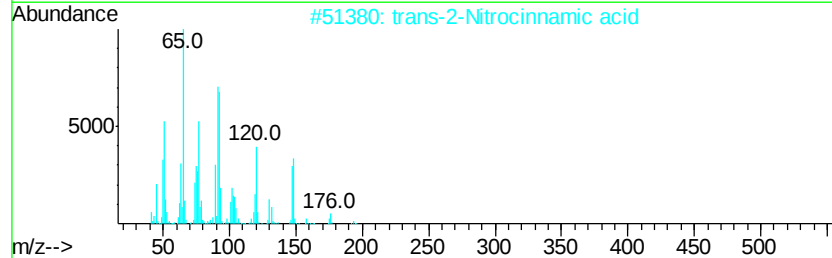
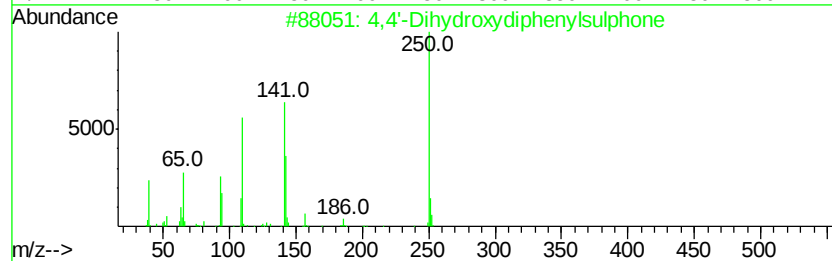
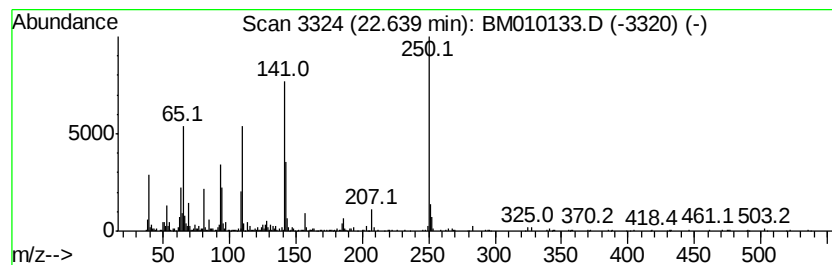
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Peak Number 5 4,4'-Dihydroxydiphenylsulphone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.64	7.36 ng	1006350	Chrysene-d12	21.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	98
2	trans-2-Nitrocinnamic acid	193	C9H7NO4	000612-41-9	22
3	Isoindole-1,3-dione, 1,3-dihydro...	345	C20H15N3O3	1000295-36-9	22
4	3-Buten-2-one, 4-(2-furanvl)-	136	C8H8O2	000623-15-4	16
5	Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	20.2	ng	892736	1	7.96	885611	20.0
unknown7.50	7.50	108.8	ng	4817230	1	7.96	885611	20.0
n-Hexadecanoic acid	18.18	2.1	ng	180973	4	17.33	1738530	20.0
4,4'-Dihydroxydip...	22.64	7.4	ng	1006350	5	21.49	2733560	20.0