

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
 Data File : BG024653.D
 Acq On : 3 Nov 2016 15:09
 Operator : UM/SJ
 Sample : H5493-26
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-6(6-8)

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-BG102516.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	3.131	44	50	70	rVB	8718745	16755505	100.00%	21.911%
2	5.334	418	425	435	rVB	561427	942323	5.62%	1.232%
3	5.798	496	504	514	rBV	2601998	4478318	26.73%	5.856%
4	7.408	769	778	789	rBV	2724221	4970119	29.66%	6.499%
5	7.796	835	844	852	rBV	2618940	4719098	28.16%	6.171%
6	8.266	916	924	932	rBV	441728	809742	4.83%	1.059%
7	8.595	972	980	992	rVB	2000389	3569761	21.31%	4.668%
8	9.441	1116	1124	1132	rBV	1655234	3088507	18.43%	4.039%
9	11.098	1396	1406	1414	rBV2	531968	1035839	6.18%	1.355%
10	13.507	1807	1816	1823	rBV	3992700	6571709	39.22%	8.594%
11	14.318	1948	1954	1961	rBV	1041134	1605730	9.58%	2.100%
12	14.882	2043	2050	2057	rVB	896396	1442219	8.61%	1.886%
13	16.368	2295	2303	2312	rBV	4131832	6486663	38.71%	8.482%
14	17.626	2510	2517	2523	rBV2	1220509	1908450	11.39%	2.496%
15	18.466	2656	2660	2667	rBV2	188771	292473	1.75%	0.382%
16	20.205	2949	2956	2964	rBV	7988792	11352121	67.75%	14.845%
17	21.497	3171	3176	3187	rBV2	295232	560472	3.35%	0.733%
18	21.762	3216	3221	3227	rVB	234353	347136	2.07%	0.454%
19	21.921	3241	3248	3257	rVB	1643916	2753487	16.43%	3.601%
20	25.346	3820	3831	3846	rVB2	912095	2781624	16.60%	3.637%

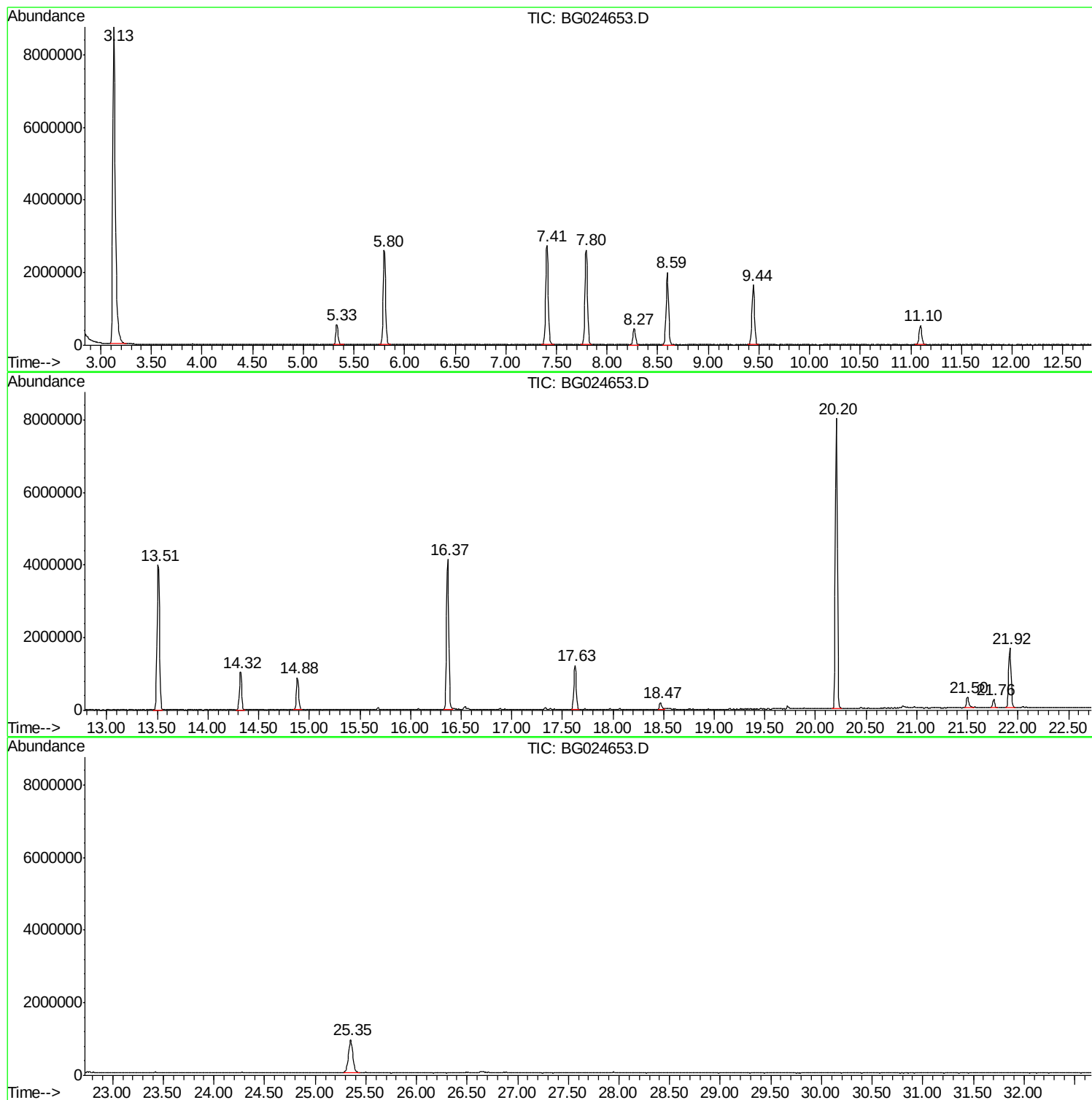
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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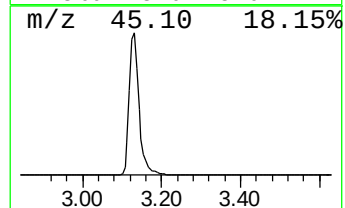
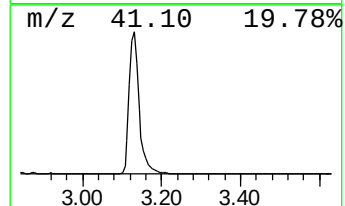
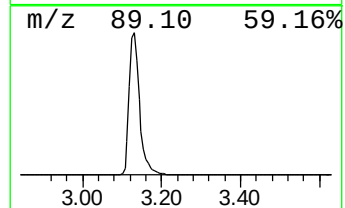
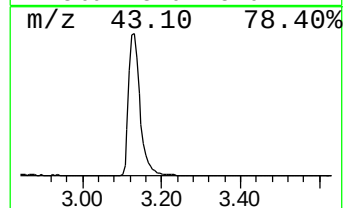
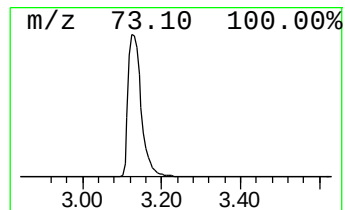
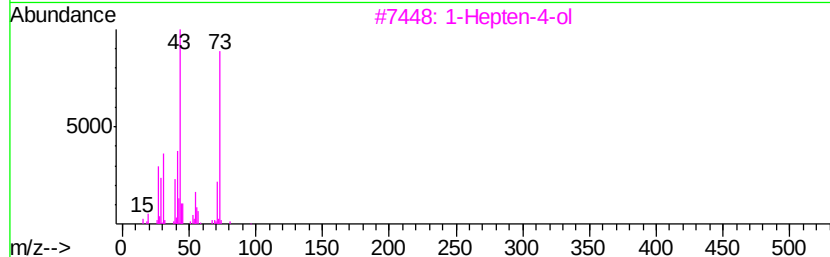
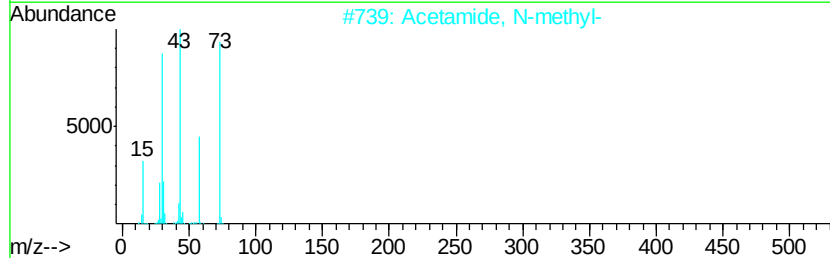
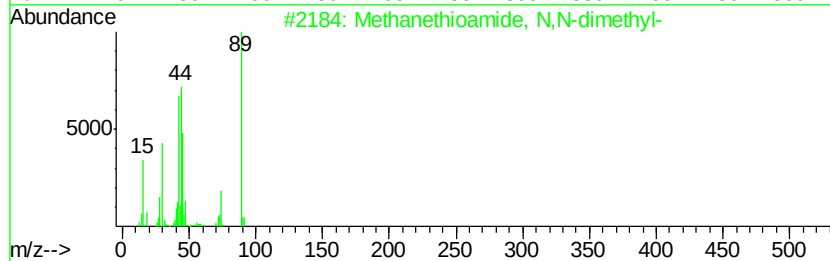
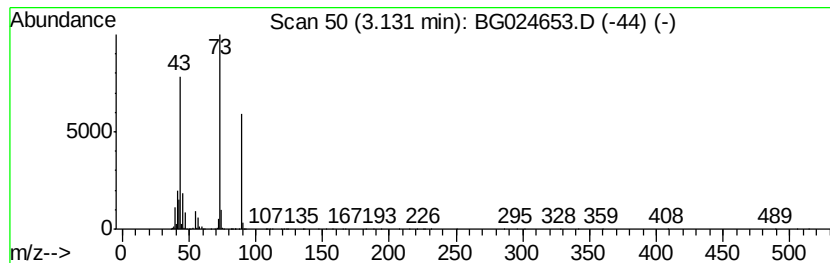
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	413.85 ng	16755500	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	40
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3		1-Hepten-4-ol	114	C7H14O	003521-91-3	23
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
5		Thiopropionamide	89	C3H7NS	000631-58-3	9



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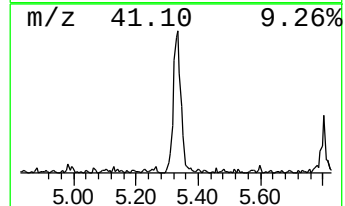
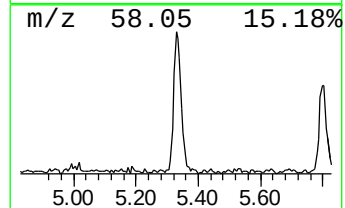
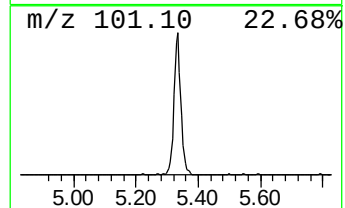
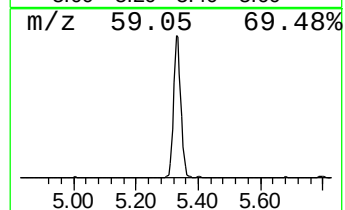
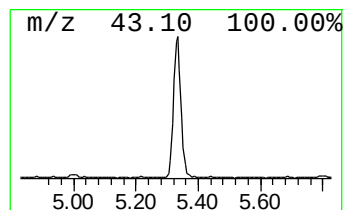
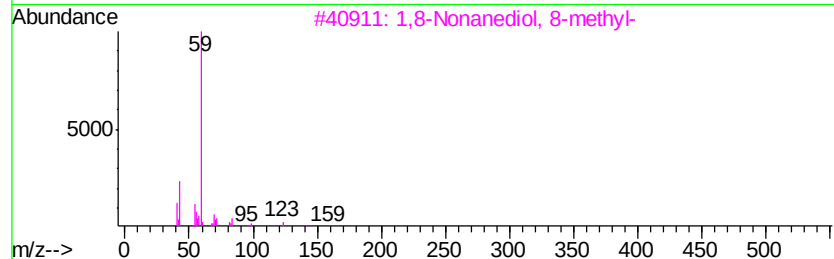
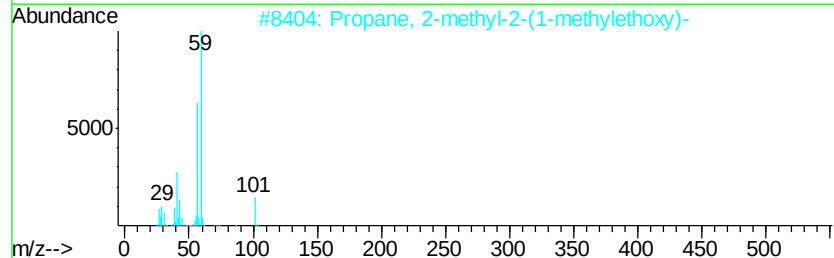
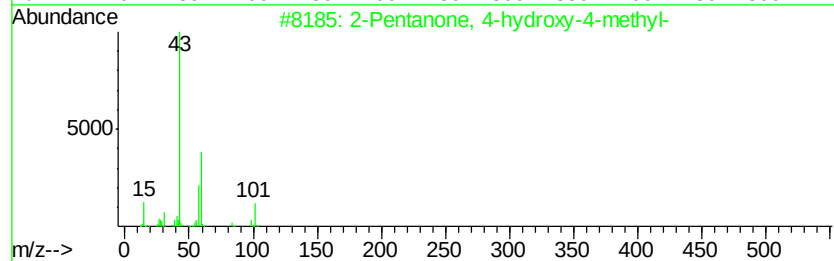
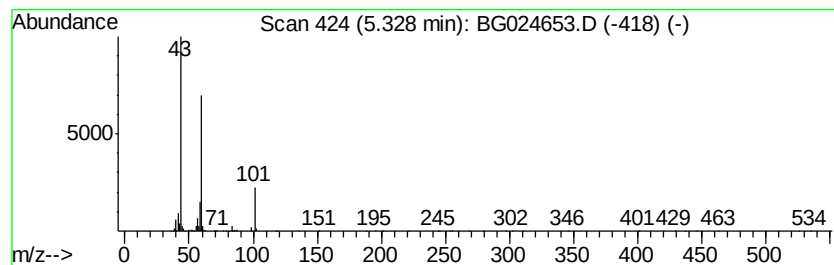
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	23.27 ng	942323	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	32
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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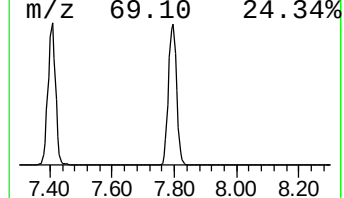
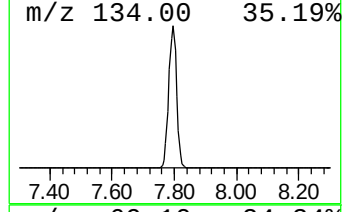
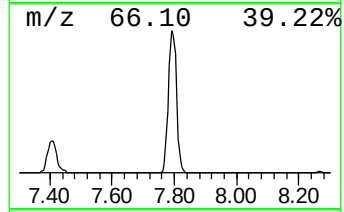
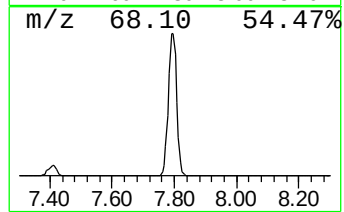
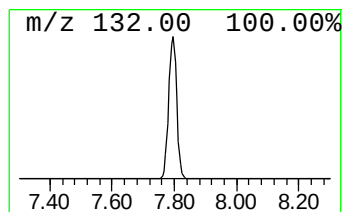
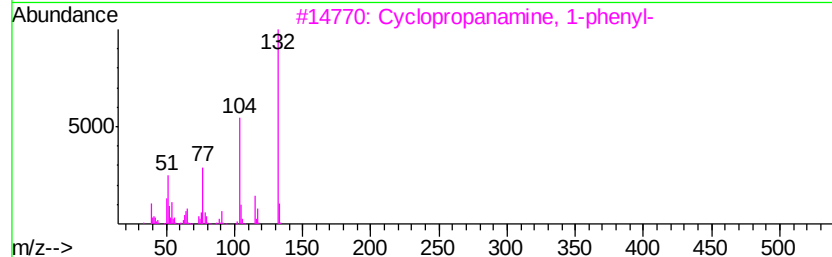
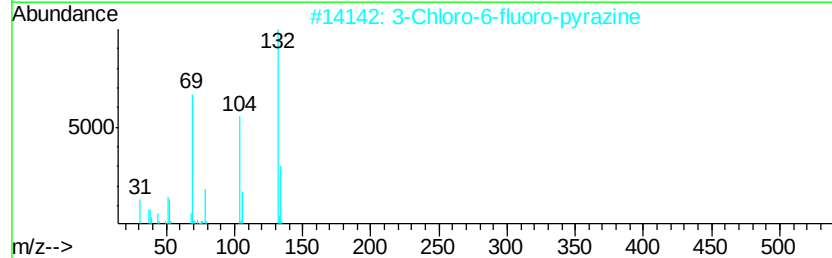
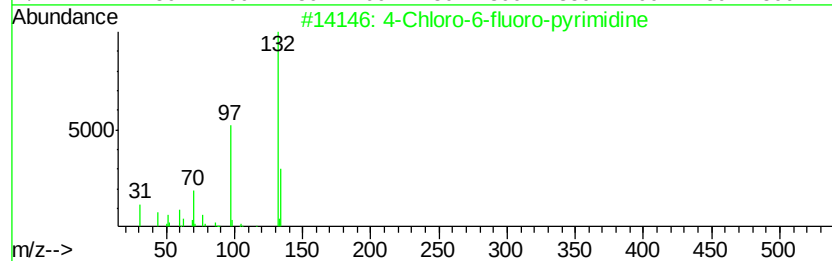
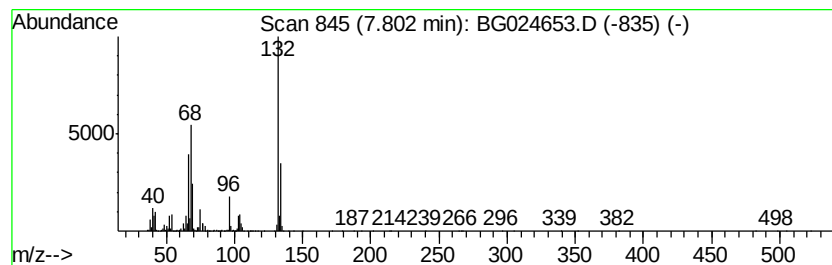
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Peak Number 3 unknown7.80 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	116.56 ng	4719100	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22



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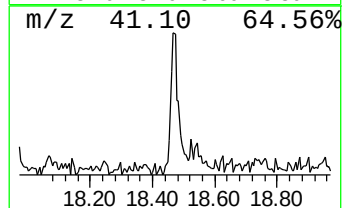
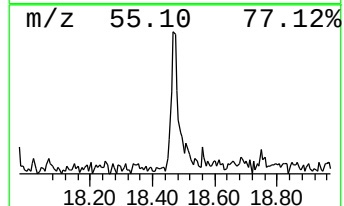
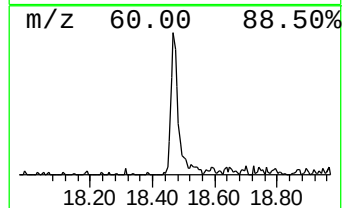
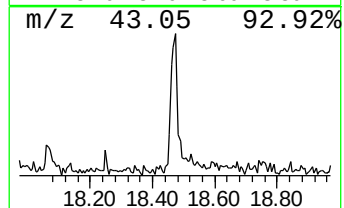
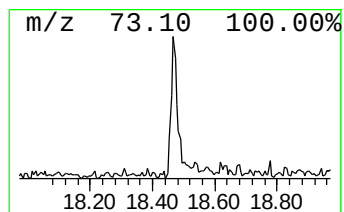
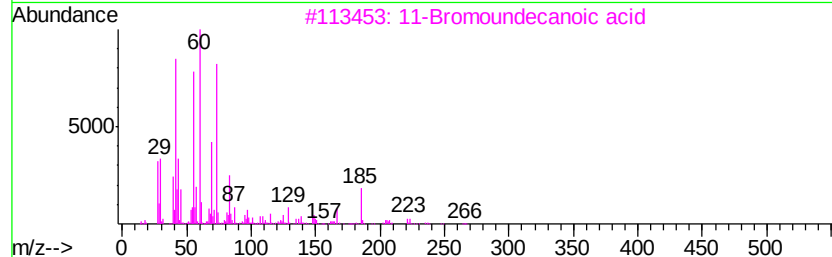
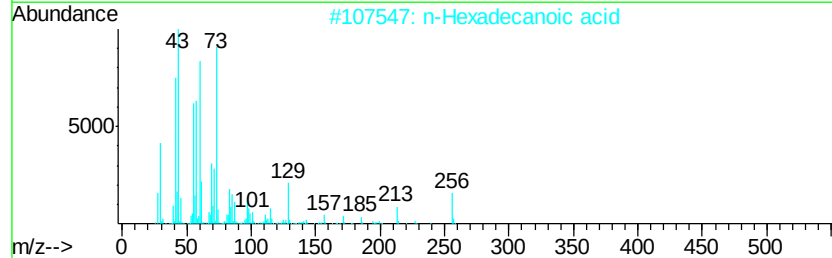
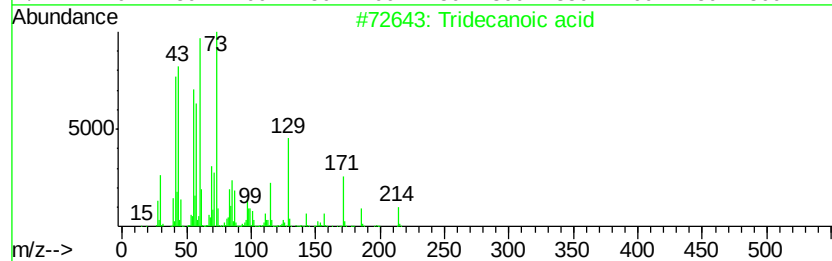
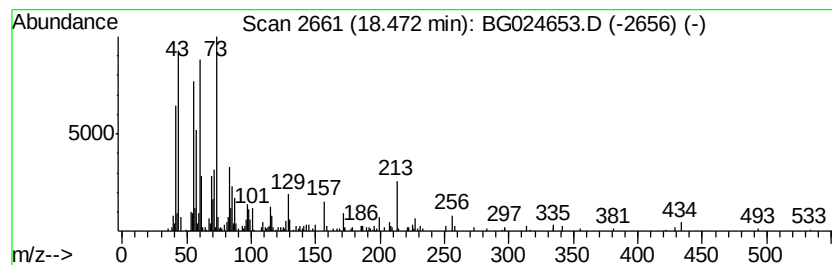
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Peak Number 5 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	3.07 ng	292473	Phenanthrene-d10	17.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	70
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	53
4		Nonanoic acid	158	C9H18O2	000112-05-0	47
5		Maltose	342	C12H22O11	000069-79-4	47



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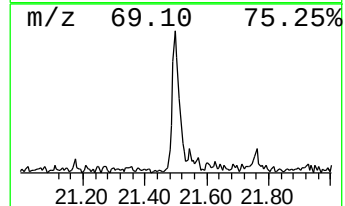
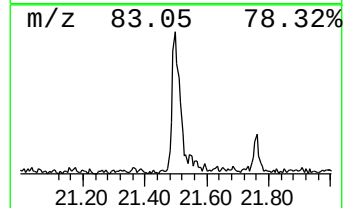
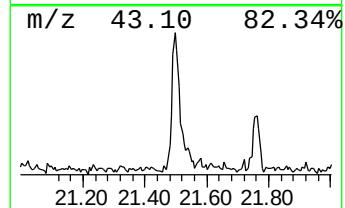
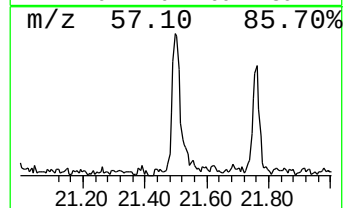
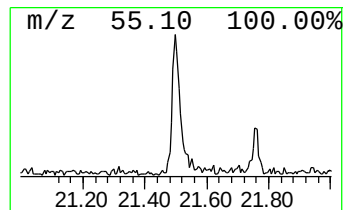
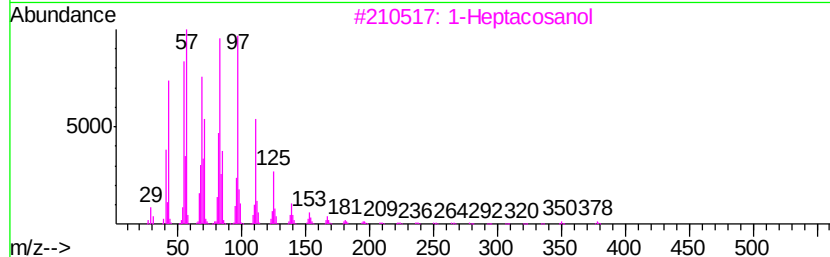
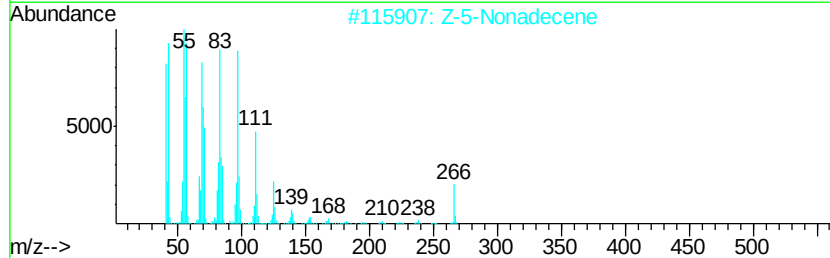
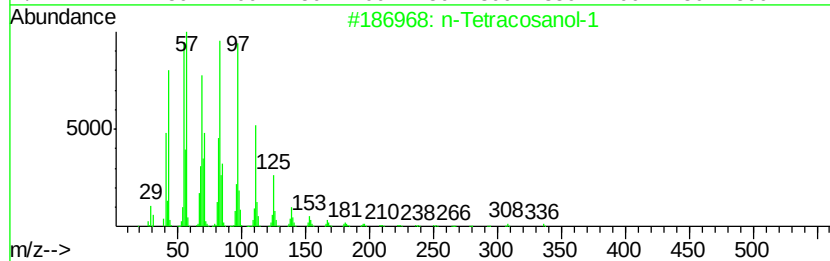
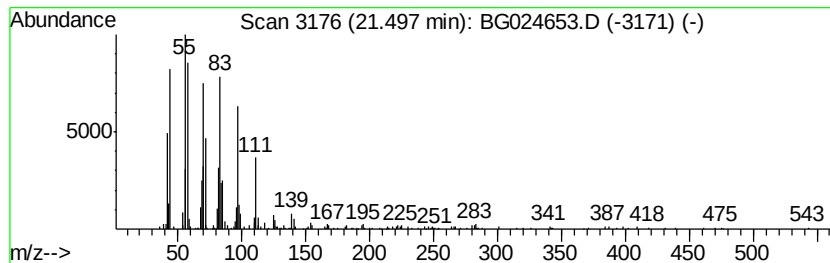
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Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.50	4.07 ng	560472	Chrysene-d12	21.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Z-5-Nonadecene	266	C19H38	1000131-11-8	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	80
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.33	23.3	ng	942323	1	8.27	809742	20.0
unknown7.80	7.80	116.6	ng	4719100	1	8.27	809742	20.0
Tridecanoic acid	18.47	3.1	ng	292473	4	17.63	1908450	20.0
n-Tetracosanol-1	21.50	4.1	ng	560472	5	21.92	2753490	20.0