

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
 Data File : BG024585.D
 Acq On : 1 Nov 2016 10:12
 Operator : UM/SJ
 Sample : H5447-05
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RPC-B2

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	3.129	43	49	66	rVB	6863292	13744610	100.00%	22.432%
2	5.332	419	424	432	rVB	490598	812857	5.91%	1.327%
3	5.802	496	504	512	rBV	2108974	3575068	26.01%	5.835%
4	7.406	769	777	787	rBV	2127681	4014105	29.20%	6.551%
5	7.794	835	843	852	rBV	2094210	3738930	27.20%	6.102%
6	8.270	915	924	933	rBV	478761	858145	6.24%	1.401%
7	8.593	970	979	990	rBV	1529849	2734366	19.89%	4.463%
8	9.445	1114	1124	1131	rBV	1295966	2389997	17.39%	3.901%
9	11.096	1397	1405	1414	rBV	599652	1130245	8.22%	1.845%
10	13.511	1807	1816	1822	rBV	3072102	5063040	36.84%	8.263%
11	14.322	1945	1954	1960	rBV	679628	1046655	7.62%	1.708%
12	14.886	2042	2050	2056	rVB	995165	1622157	11.80%	2.648%
13	16.366	2295	2302	2310	rBV	2928213	4619020	33.61%	7.539%
14	17.624	2506	2516	2524	rBV	1310197	2056266	14.96%	3.356%
15	20.203	2948	2955	2962	rBV	5772264	7836338	57.01%	12.790%
16	21.496	3170	3175	3183	rBV5	154917	276469	2.01%	0.451%
17	21.919	3240	3247	3254	rVB	1544159	2727093	19.84%	4.451%
18	23.435	3498	3505	3512	rBV4	81436	195472	1.42%	0.319%
19	25.350	3817	3831	3844	rVB2	907438	2830410	20.59%	4.619%

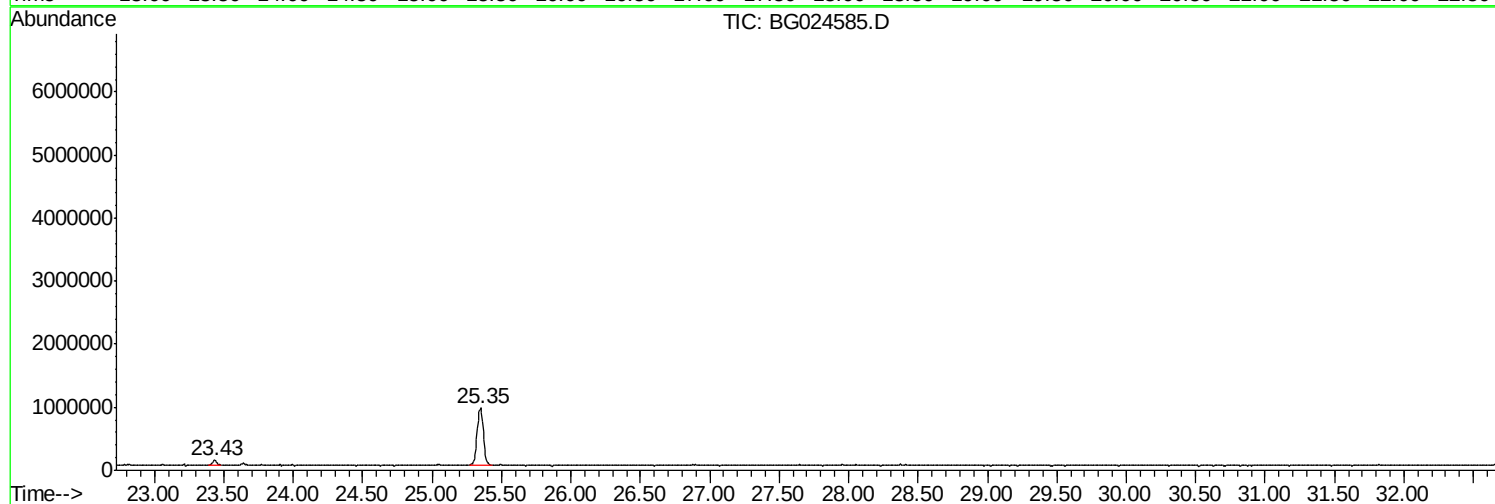
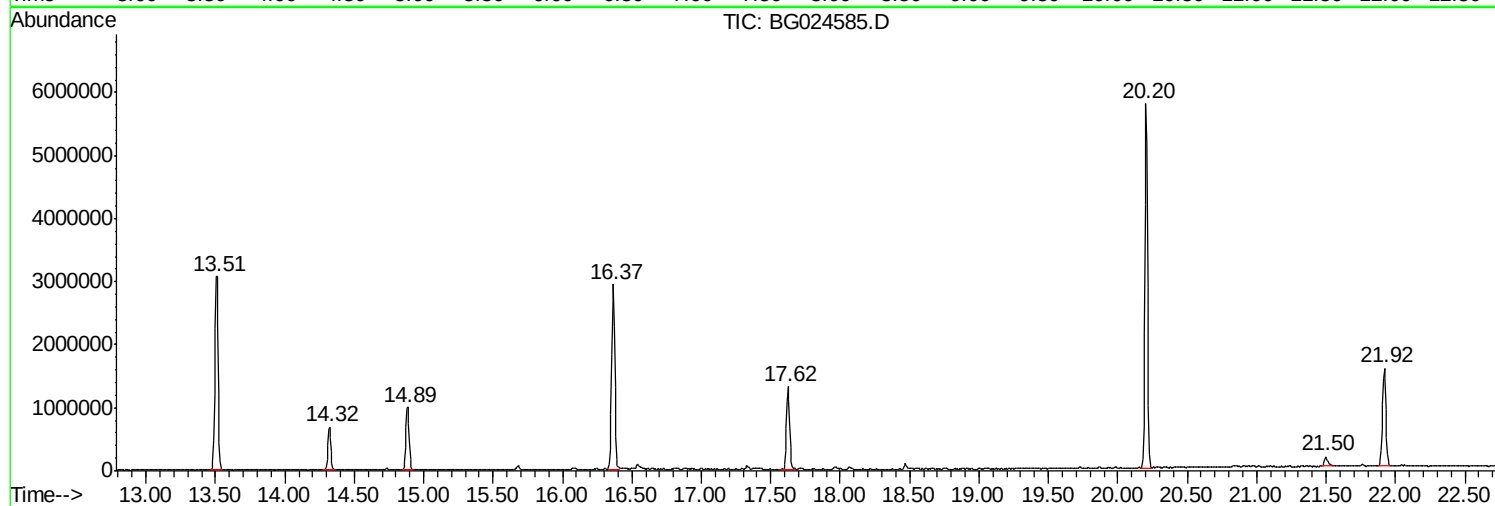
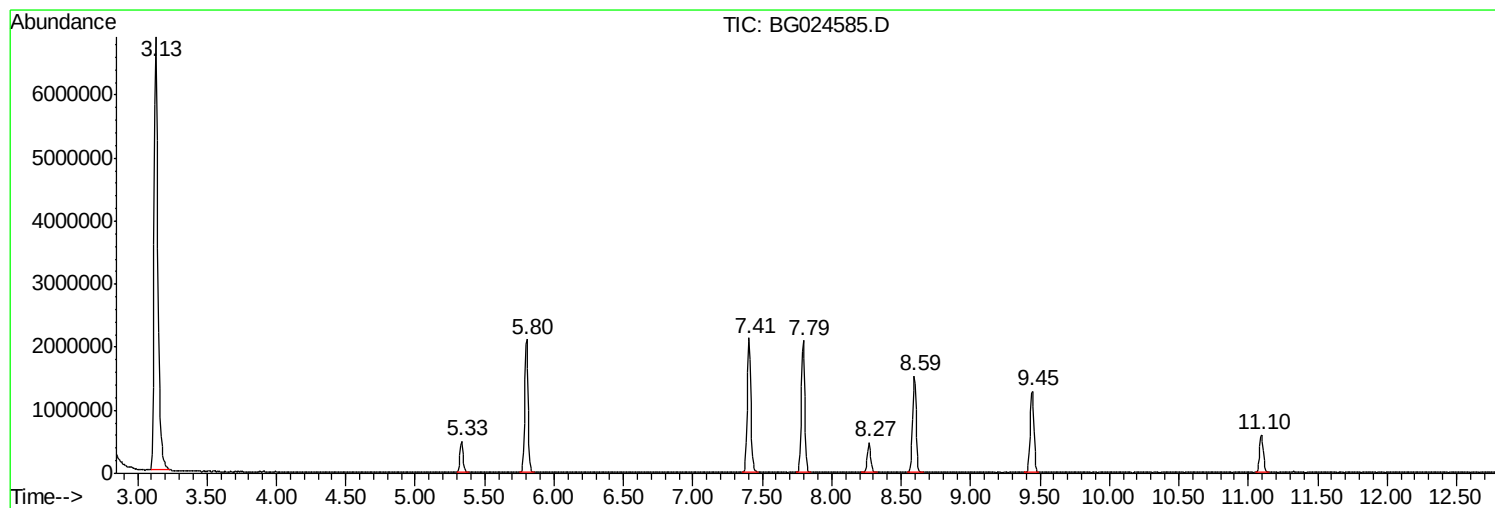
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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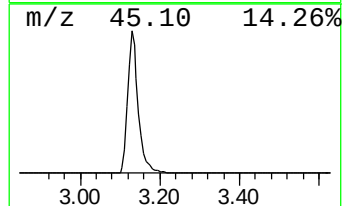
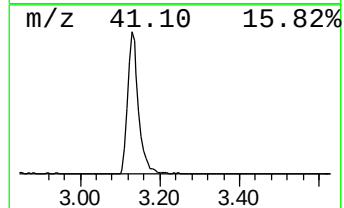
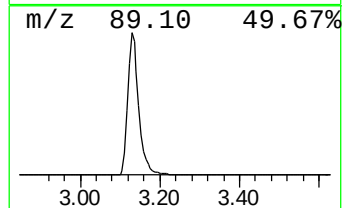
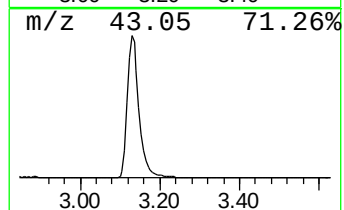
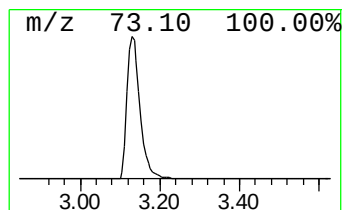
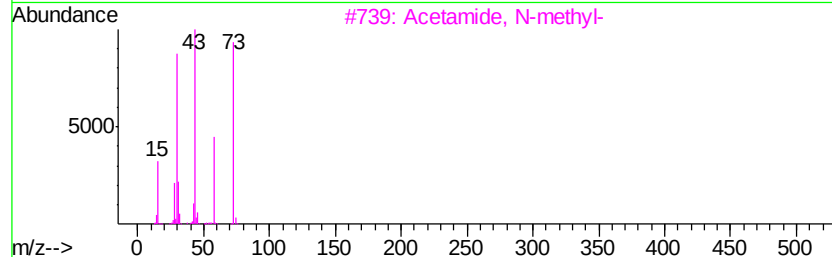
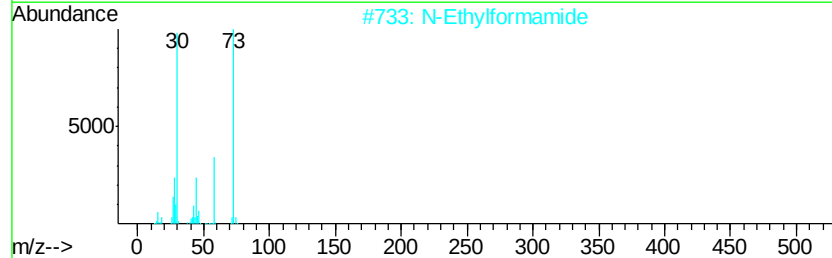
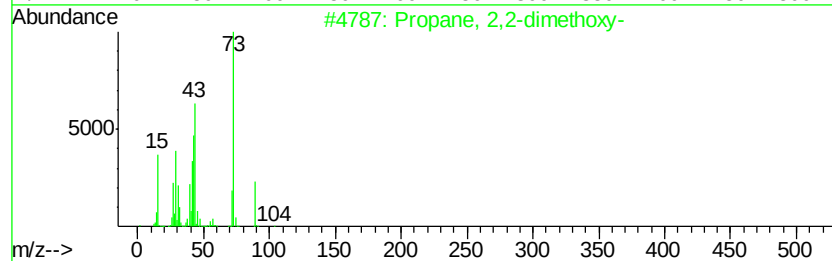
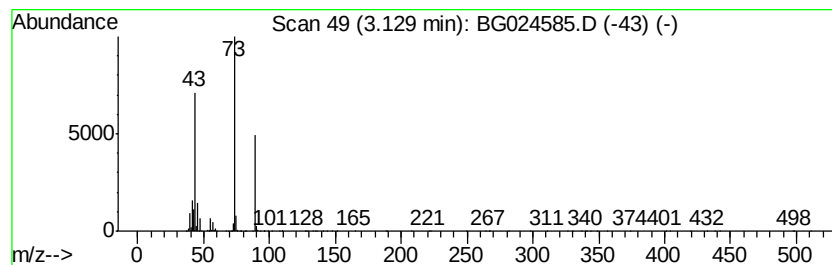
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	320.33 ng	13744600	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5		1-Hepten-4-ol	114	C7H14O	003521-91-3	9



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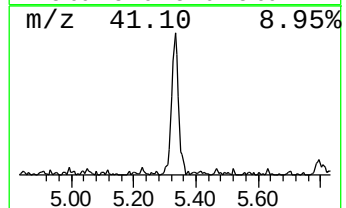
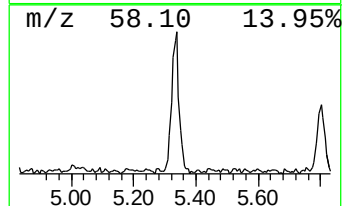
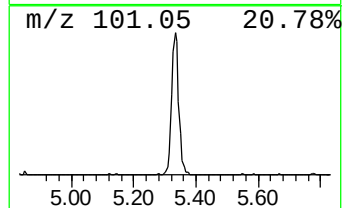
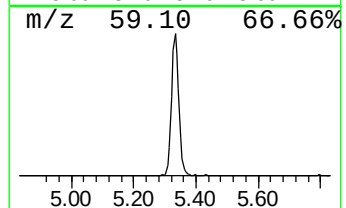
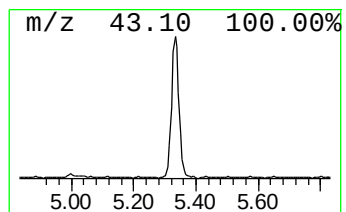
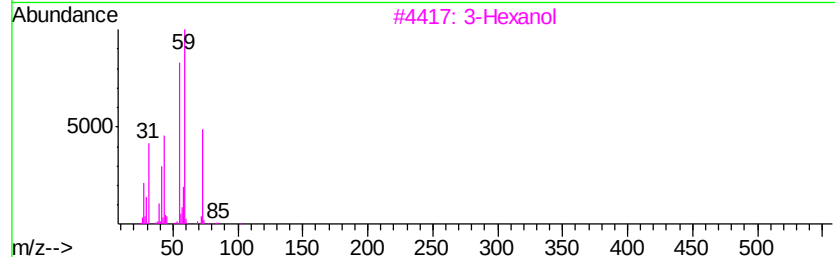
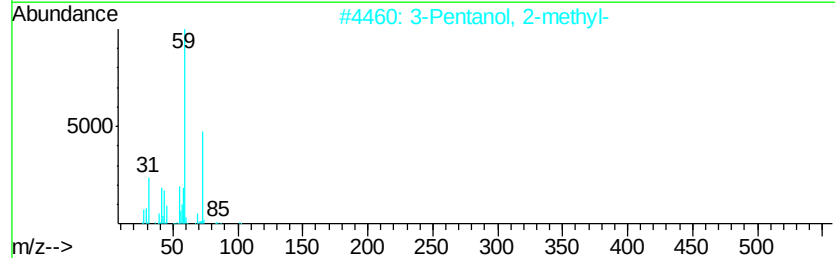
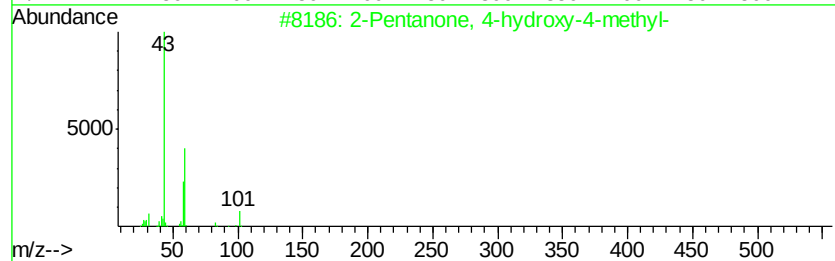
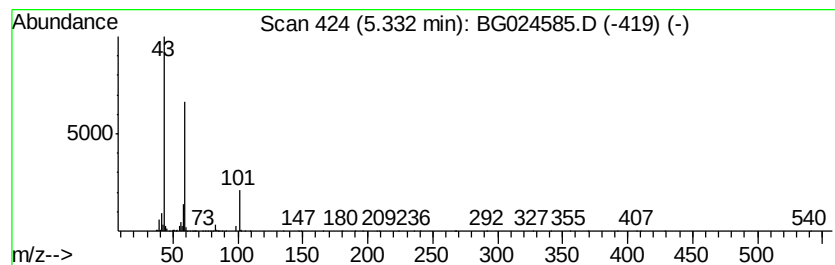
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	18.94 ng	812857	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	50
2		3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	43
3		3-Hexanol	102	C6H14O	000623-37-0	25
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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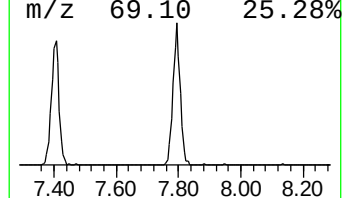
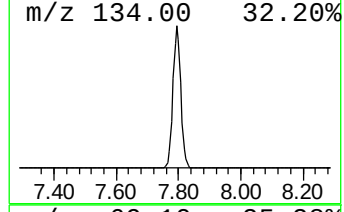
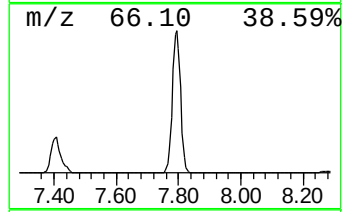
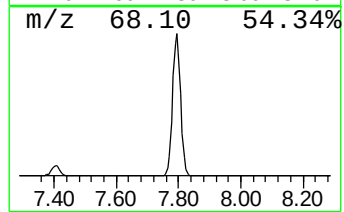
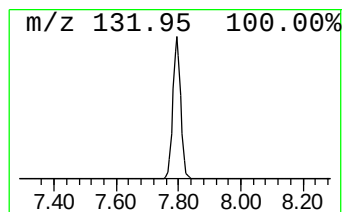
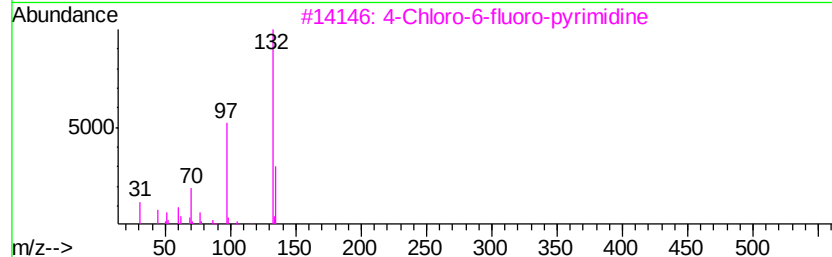
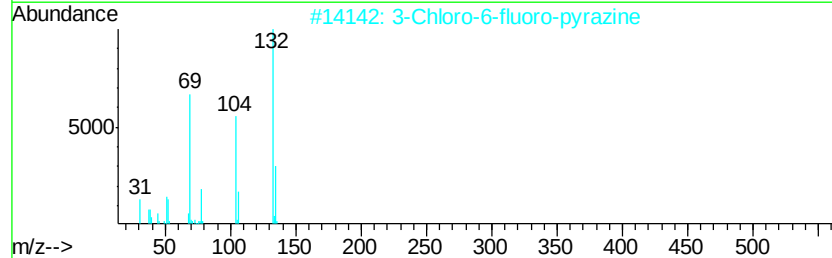
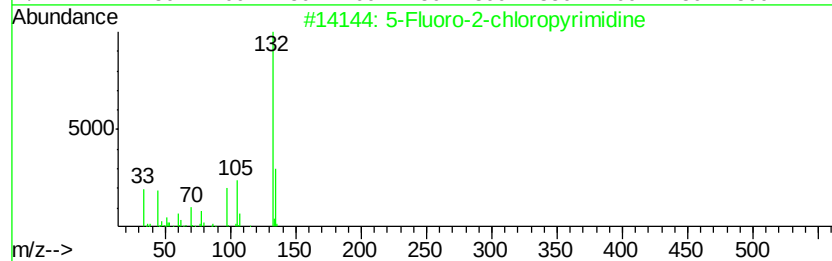
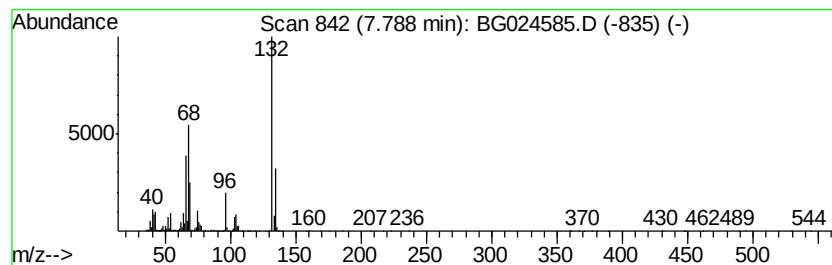
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Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	87.14 ng	3738930	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
5		5-Aminoindole	132	C8H8N2	005192-03-0	22



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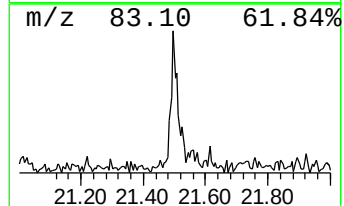
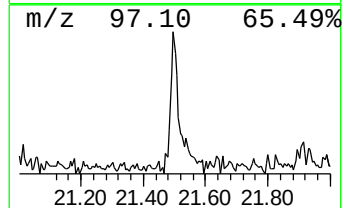
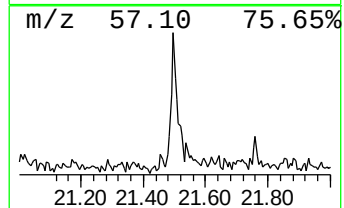
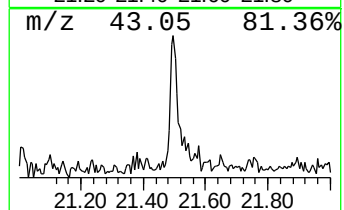
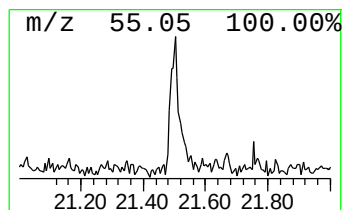
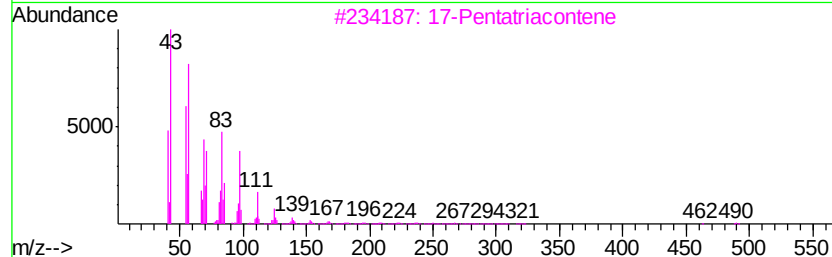
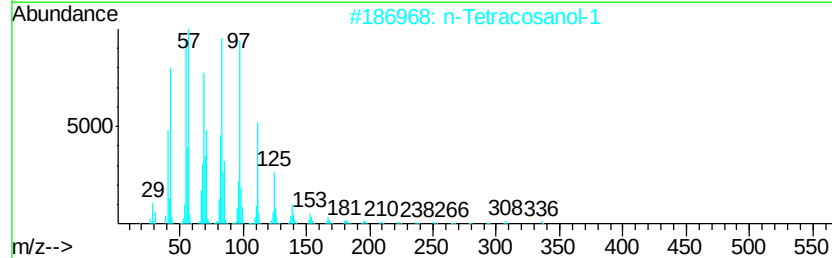
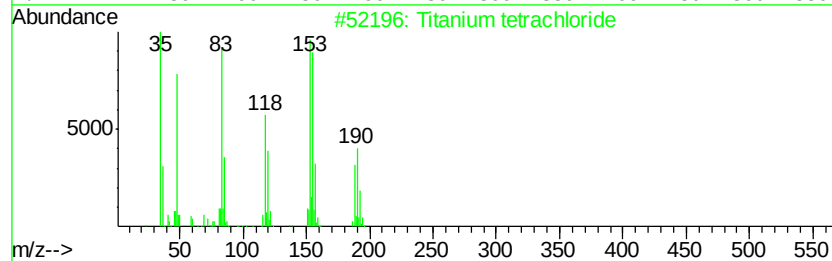
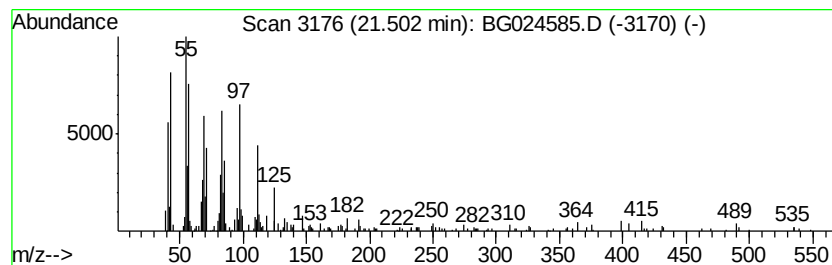
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Peak Number 5 Titanium tetrachloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
21.50	2.03 ng	276469	Chrysene-d12		21.92
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Titanium tetrachloride	188	Cl4Ti	007550-45-0	70
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
3	17-Pentatriacontene	491	C35H70	006971-40-0	70
4	Behenic alcohol	326	C22H46O	000661-19-8	64
5	Cyclotetracosane	336	C24H48	000297-03-0	53



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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	18.9	ng	812857	1	8.27	858145	20.0
unknown7.79	7.79	87.1	ng	3738930	1	8.27	858145	20.0
Titanium tetrachl...	21.50	2.0	ng	276469	5	21.92	2727090	20.0