

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
 Data File : BG043404.D
 Acq On : 30 Oct 2019 17:19
 Operator : JU
 Sample : PB124338BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB124338BL

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_G\METHODS\8270-BG102119.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	5.122	341	346	355	rBV	104060	166780	4.92%	1.063%
2	5.609	421	429	441	rBV	532606	927062	27.37%	5.909%
3	7.207	693	701	718	rBV	544669	1026185	30.30%	6.541%
4	7.566	753	762	775	rBV	562210	1038744	30.67%	6.621%
5	8.018	831	839	849	rBV	123789	224596	6.63%	1.432%
6	8.347	887	895	910	rBV	447676	823027	24.30%	5.246%
7	9.182	1027	1037	1049	rBV	275954	588375	17.37%	3.750%
8	10.827	1310	1317	1330	rBV	125097	273911	8.09%	1.746%
9	13.271	1726	1733	1749	rBV	909443	1616072	47.72%	10.301%
10	14.652	1961	1968	1980	rBV	253267	452527	13.36%	2.884%
11	16.138	2214	2221	2232	rBV	872987	1510249	44.59%	9.627%
12	17.395	2428	2435	2451	rBV2	330661	629149	18.58%	4.010%
13	20.004	2872	2879	2896	rBV	2450483	3386651	100.00%	21.587%
14	21.256	3085	3092	3097	rBV	88185	178790	5.28%	1.140%
15	21.320	3097	3103	3108	rVV	144006	242695	7.17%	1.547%
16	21.379	3108	3113	3123	rVV	399056	657267	19.41%	4.189%
17	21.461	3124	3127	3135	rVB2	24457	44097	1.30%	0.281%
18	21.661	3152	3161	3173	rBV2	442247	859841	25.39%	5.481%
19	23.130	3406	3411	3418	rVB3	21676	43630	1.29%	0.278%
20	23.929	3541	3547	3555	rVB5	28944	65672	1.94%	0.419%
21	24.857	3694	3705	3721	rBV3	294117	933125	27.55%	5.948%

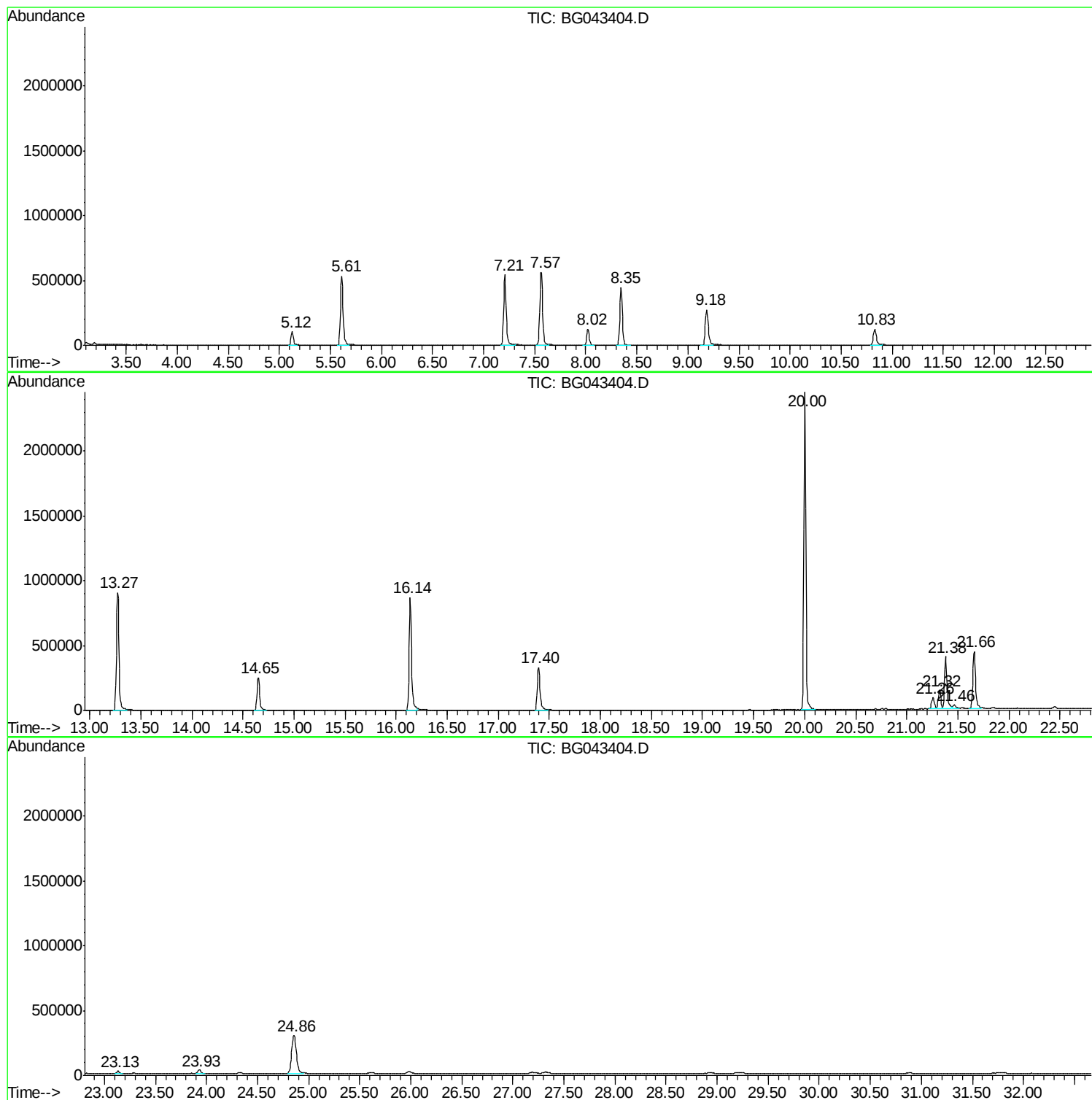
Sum of corrected areas: 15688445

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.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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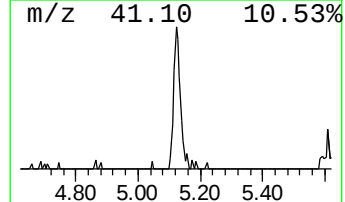
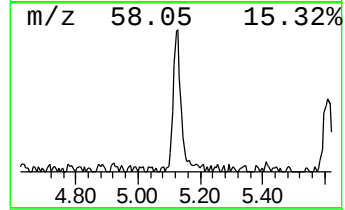
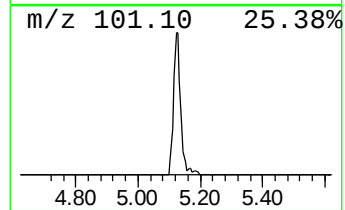
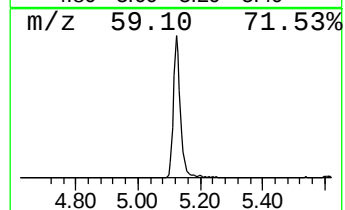
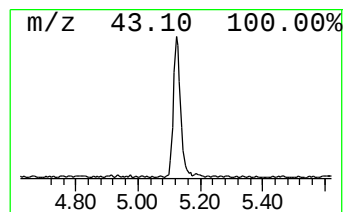
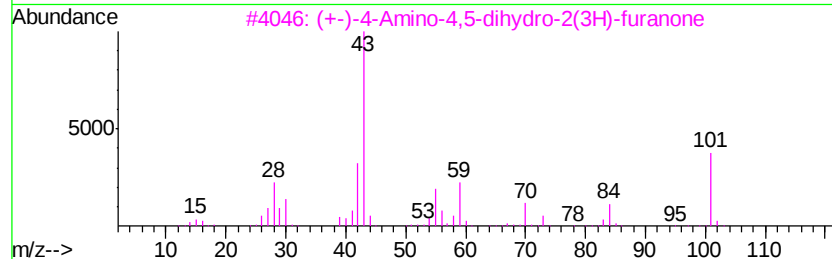
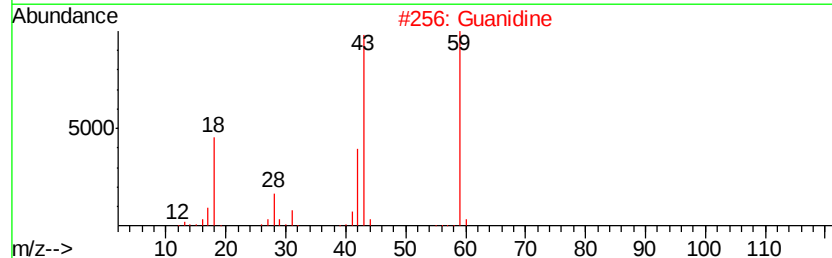
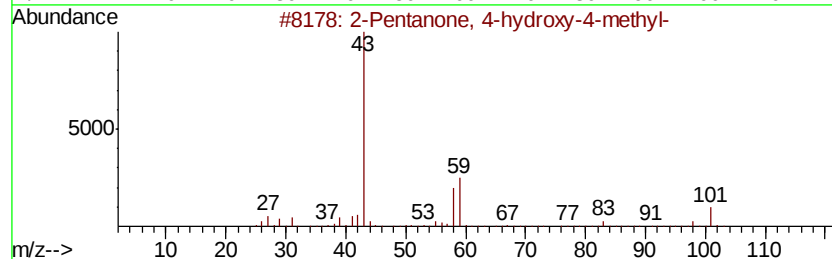
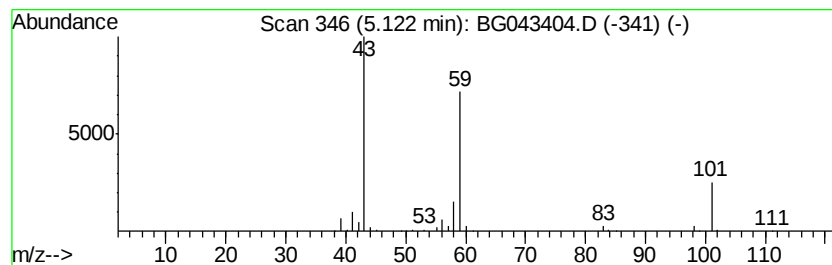
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	14.85 ng	166780	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Guanidine	59	CH5N3	000113-00-8	43
3		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	40
4		1,2-Butanediol	90	C4H10O2	000584-03-2	37
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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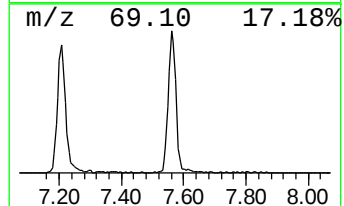
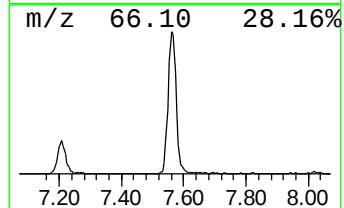
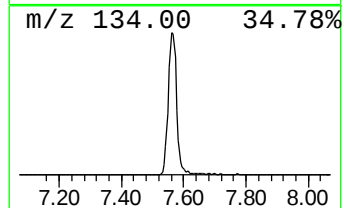
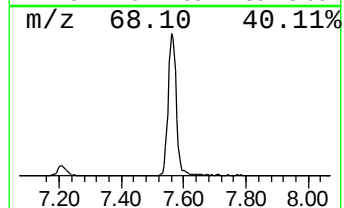
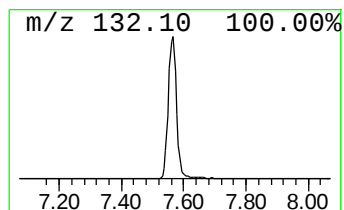
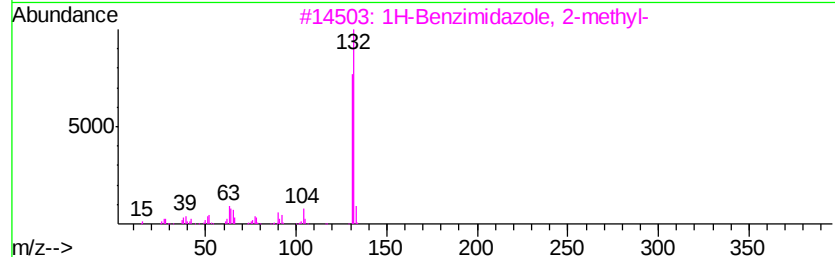
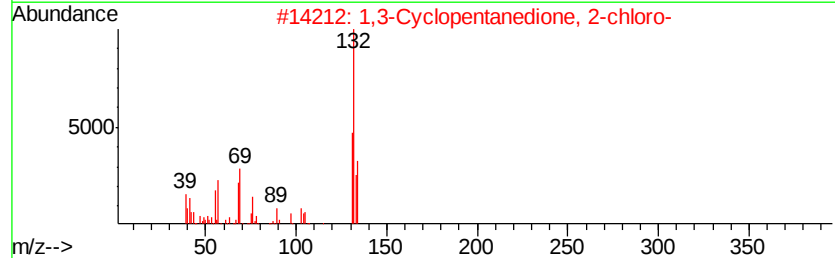
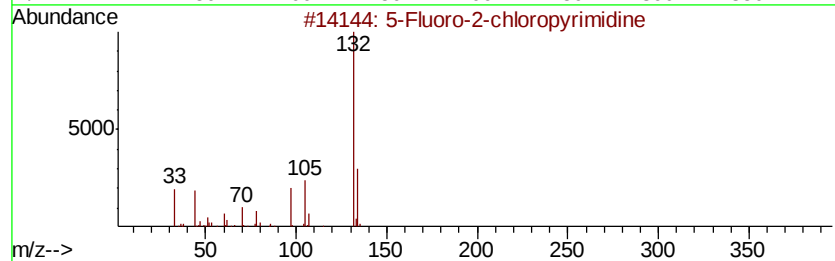
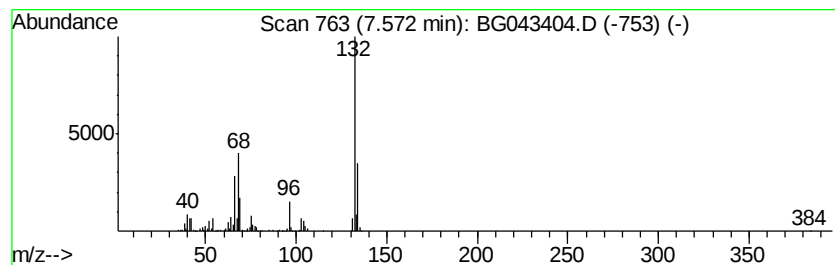
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Peak Number 2 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	92.50 ng	1038740	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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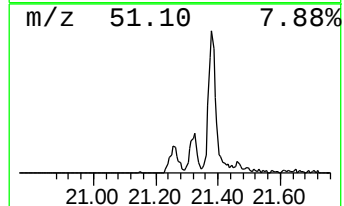
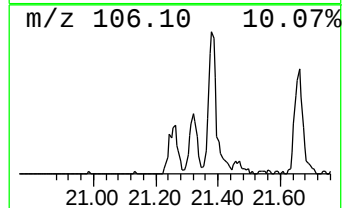
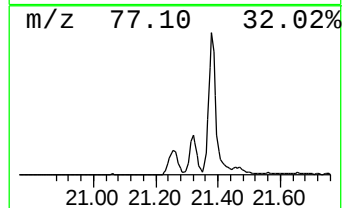
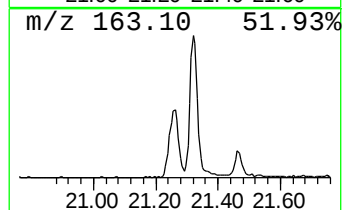
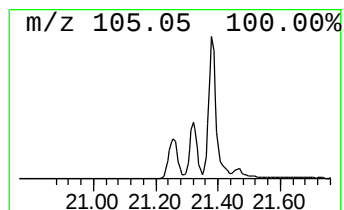
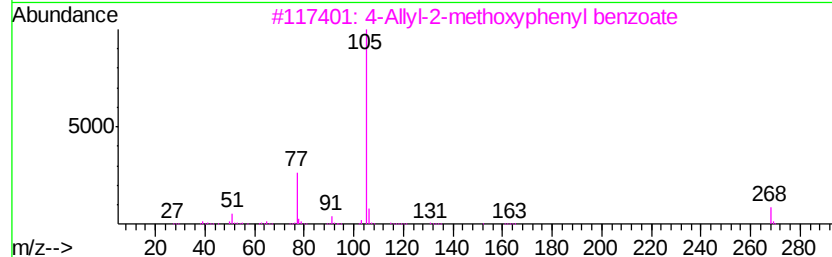
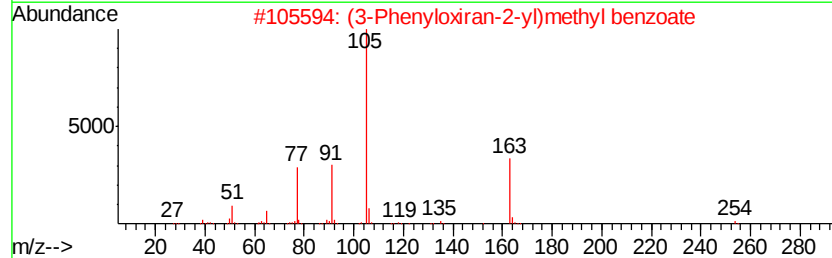
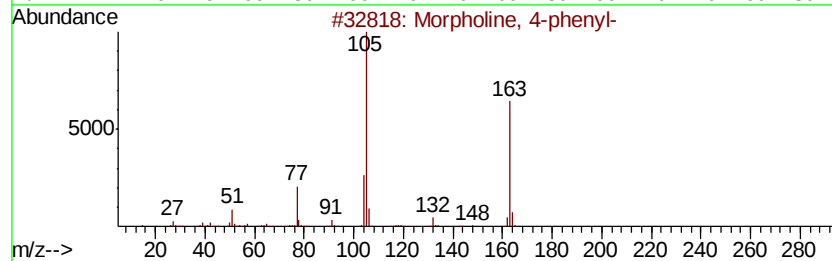
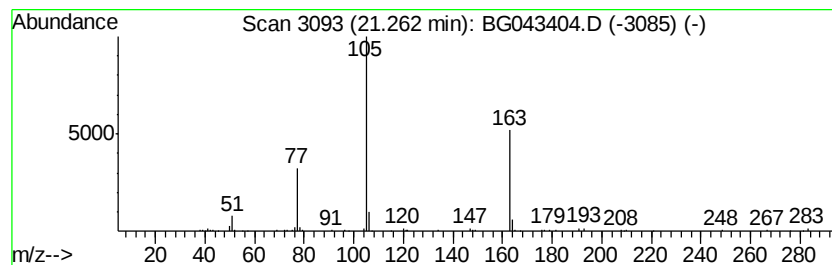
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Peak Number 4 Morpholine, 4-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.26	4.16 ng	178790	Chrysene-d12	21.66	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
2	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	56
3	4-Allyl-2-methoxyphenyl benzoate	268	C17H16O3	1000366-95-9	35
4	Glyoxylic acid, phenyl-, (2'-ace...	268	C16H12O4	166538-12-1	35
5	1,3-Phenylenedibenzoate	318	C20H14O4	000094-01-9	27



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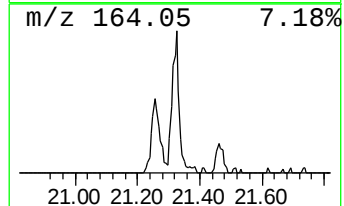
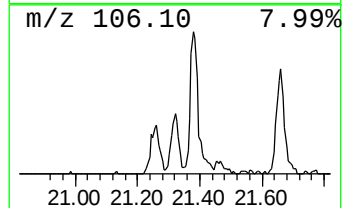
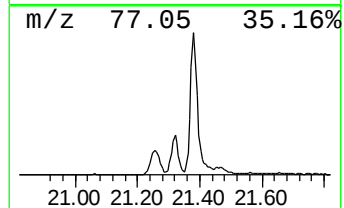
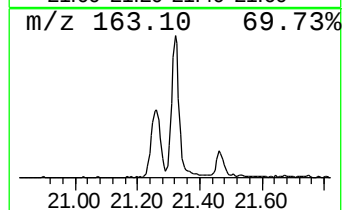
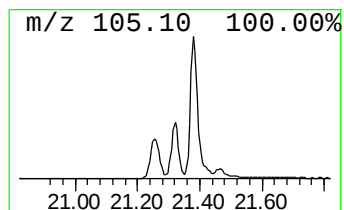
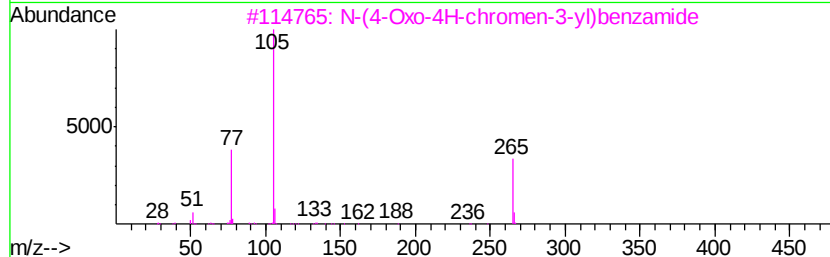
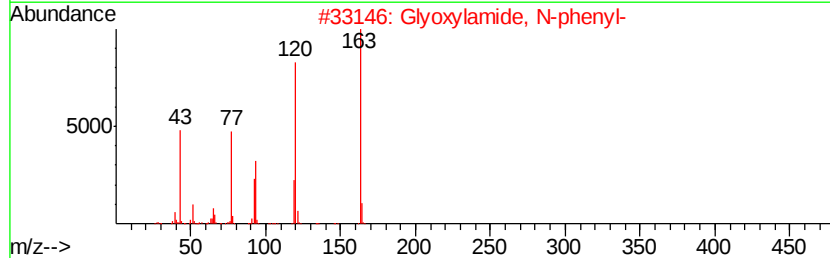
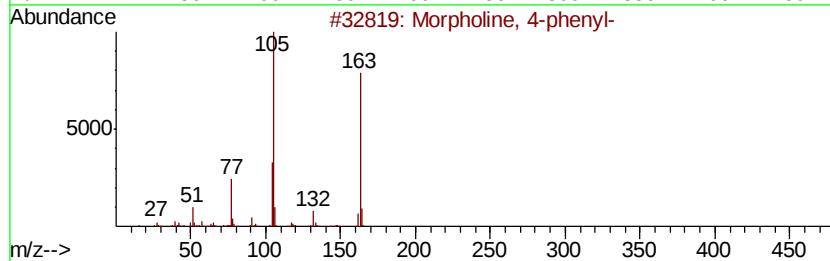
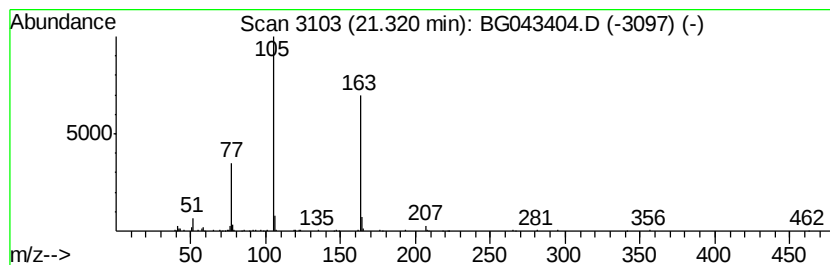
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Peak Number 5 unknown21.32 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	5.65 ng	242695	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2		Glyoxylamide, N-phenyl-	163	C9H9N02	032331-52-5	47
3		N-(4-Oxo-4H-chromen-3-yl)benzamide	265	C16H11N03	1000243-49-5	35
4		Propanoic acid, 2-(benzoylamino)...	251	C13H17N04	141627-52-3	35
5		Phthalic acid, 3,5-dimethylpheny...	284	C17H16O4	1000315-70-8	32



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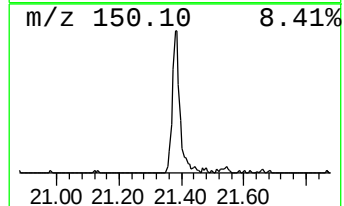
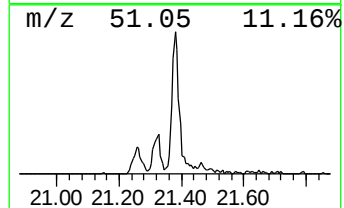
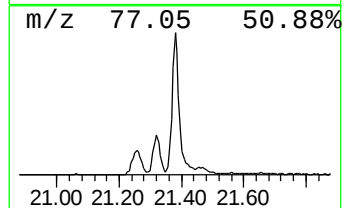
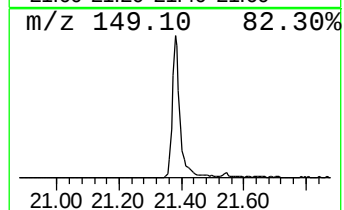
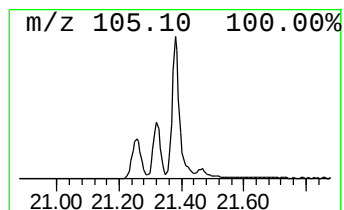
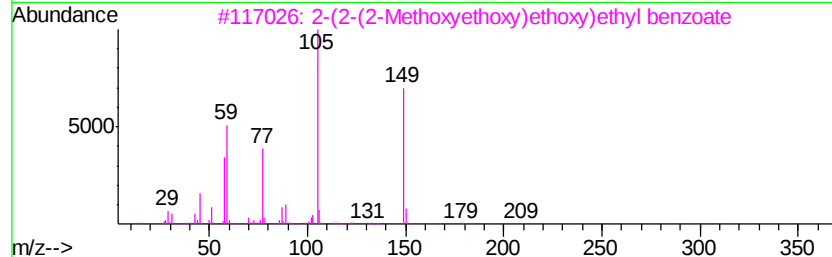
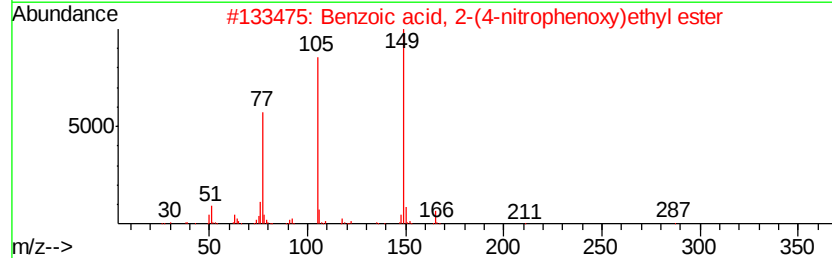
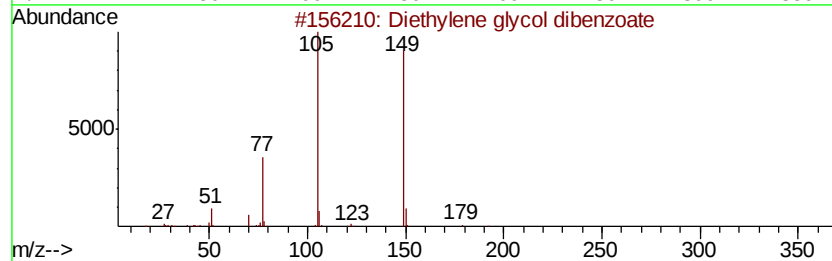
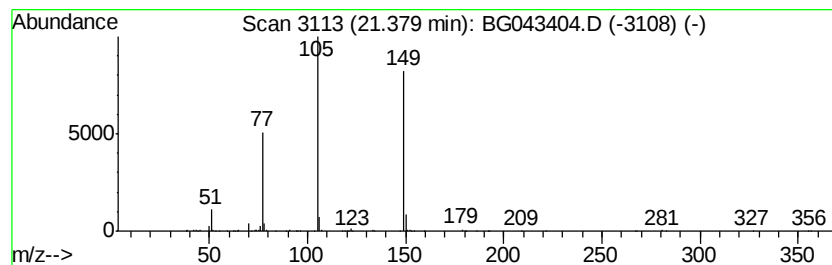
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Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	15.29 ng	657267	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2		Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
3		2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
4		3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	72
5		1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	14.9	ng	166780	1	8.02	224596	20.0
unknown7.57	7.57	92.5	ng	1038740	1	8.02	224596	20.0
Morpholine, 4-phe...	21.26	4.2	ng	178790	5	21.66	859841	20.0
unknown21.32	21.32	5.7	ng	242695	5	21.66	859841	20.0
Diethylene glycol...	21.38	15.3	ng	657267	5	21.66	859841	20.0