

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101817\
 Data File : BG029347.D
 Acq On : 19 Oct 2017 1:10
 Operator : SJ/JU
 Sample : I5836-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ENV-125-5(10-15)

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-BG101617.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	5.244	326	333	340	rBV	214558	315702	6.12%	1.189%
2	5.719	407	414	424	rBV	1132553	1796596	34.80%	6.766%
3	7.323	678	687	698	rBV	1098930	2062800	39.96%	7.769%
4	7.699	743	751	762	rBV	1104809	1914171	37.08%	7.209%
5	8.169	823	831	837	rBV	209082	363552	7.04%	1.369%
6	8.493	877	886	895	rBV	815277	1415622	27.42%	5.331%
7	9.333	1020	1029	1038	rBV	655725	1169794	22.66%	4.405%
8	10.984	1302	1310	1317	rBV	305921	547638	10.61%	2.062%
9	13.410	1716	1723	1732	rVB	1900850	2955914	57.26%	11.132%
10	14.227	1856	1862	1868	rBV	355608	508115	9.84%	1.914%
11	14.785	1948	1957	1966	rVB2	541604	846585	16.40%	3.188%
12	16.125	2177	2185	2192	rBV	64009	93494	1.81%	0.352%
13	16.266	2202	2209	2220	rBV	1894918	2825016	54.73%	10.639%
14	17.523	2416	2423	2429	rBV	806154	1197900	23.21%	4.511%
15	18.387	2564	2570	2582	rBV2	82171	152879	2.96%	0.576%
16	20.114	2857	2864	2874	rVB	3856425	5161961	100.00%	19.440%
17	21.789	3142	3149	3159	rBV	874520	1496530	28.99%	5.636%
18	23.287	3398	3404	3415	rBV3	125937	262879	5.09%	0.990%
19	25.097	3702	3712	3724	rVB2	500784	1465985	28.40%	5.521%

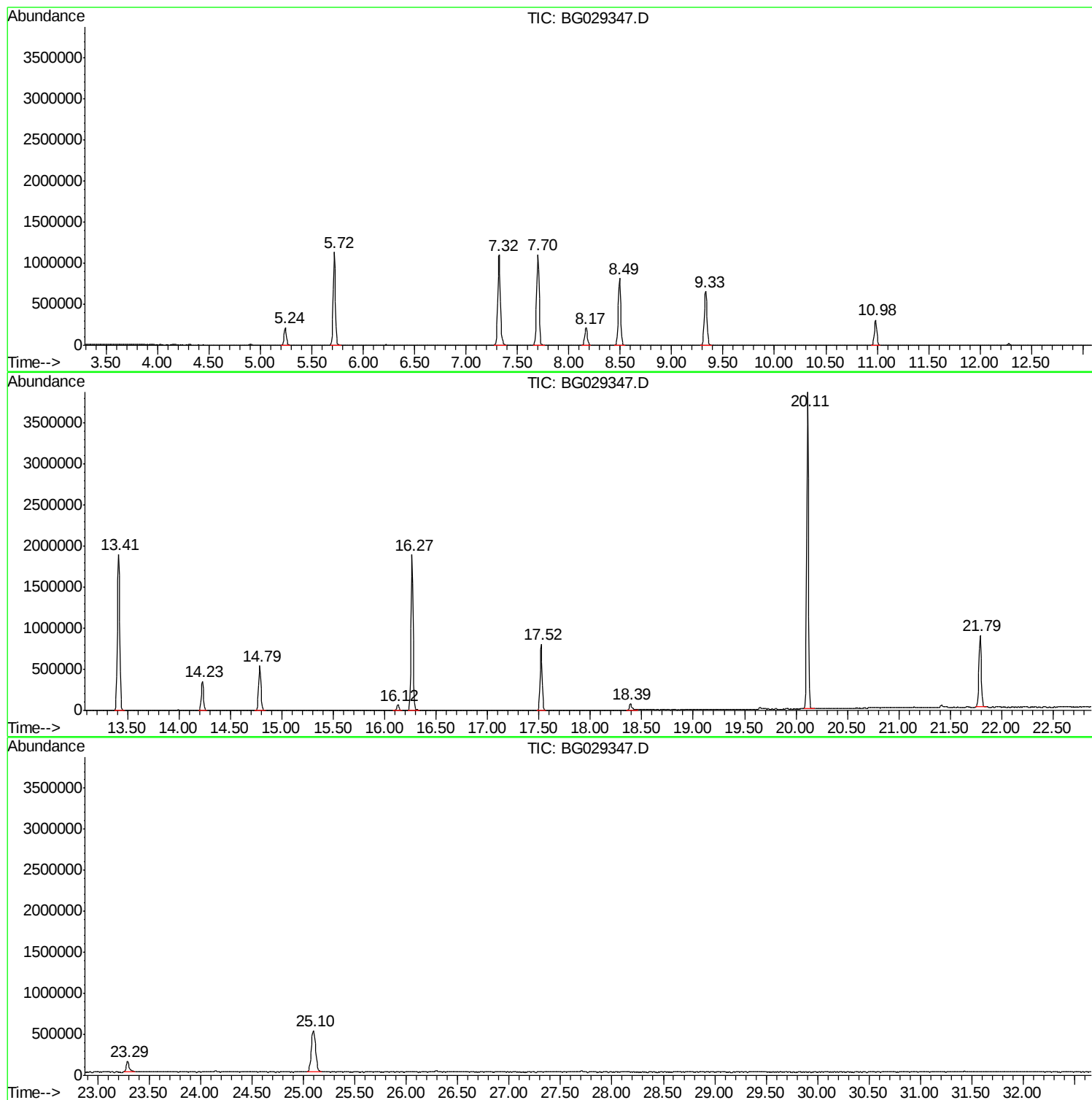
Sum of corrected areas: 26553133

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.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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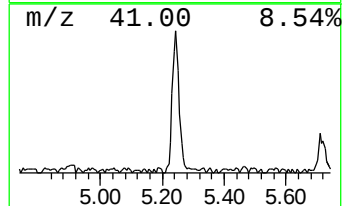
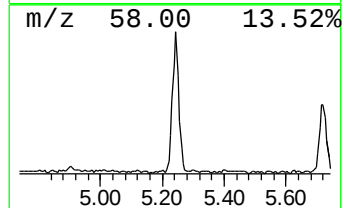
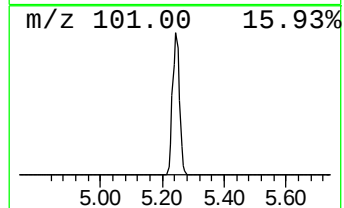
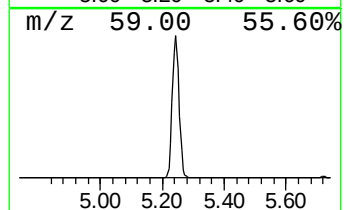
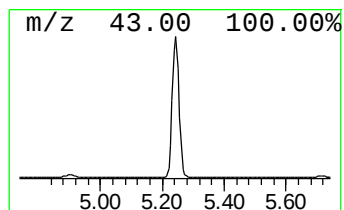
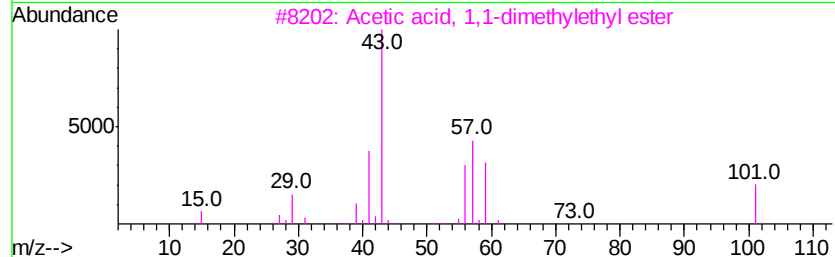
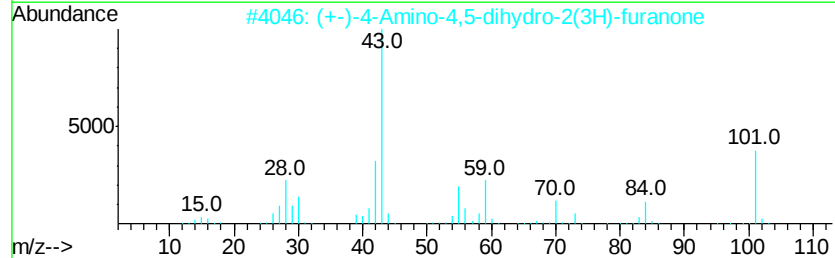
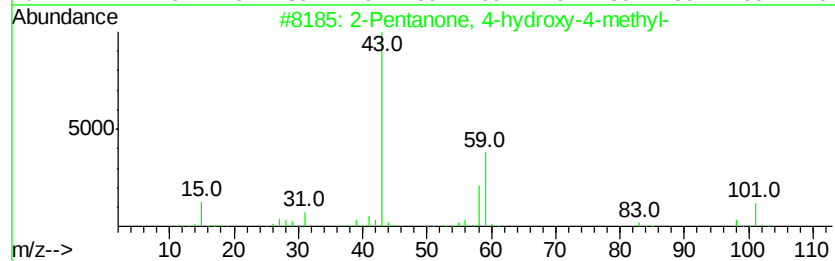
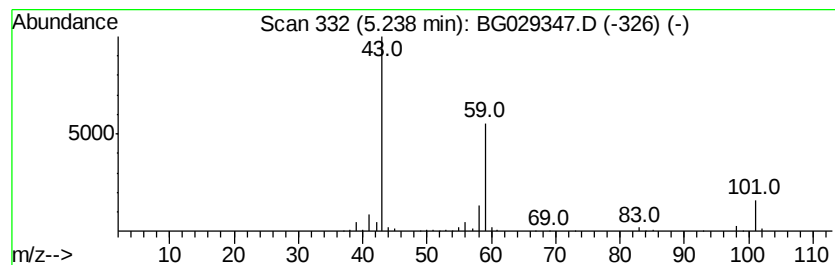
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	17.37 ng	315702	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
3		Acetic acid, 1,1-dimethylethyl ester	116	C6H12O2	000540-88-5	9
4		2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9
5		1,2-Butanediol	90	C4H10O2	000584-03-2	9



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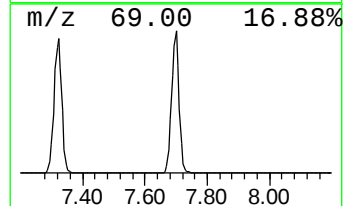
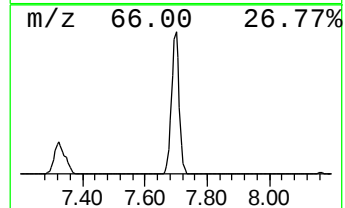
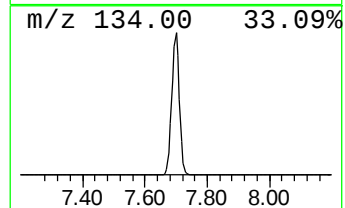
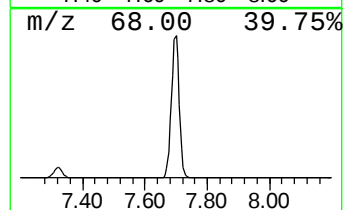
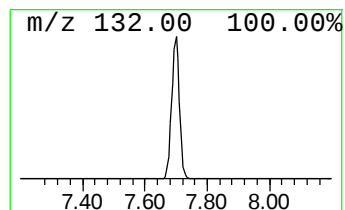
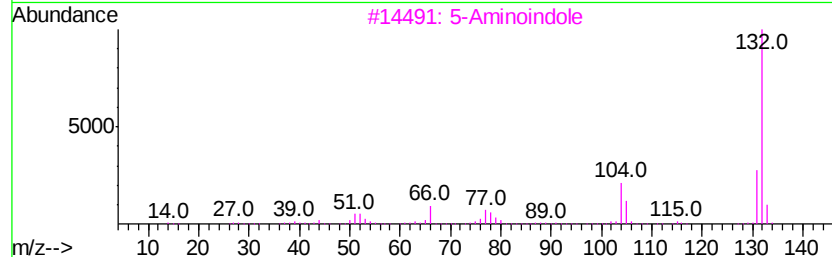
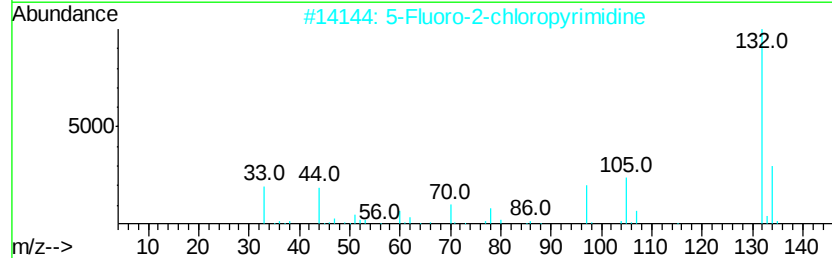
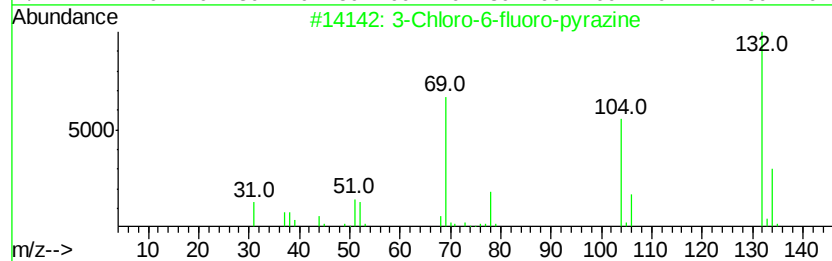
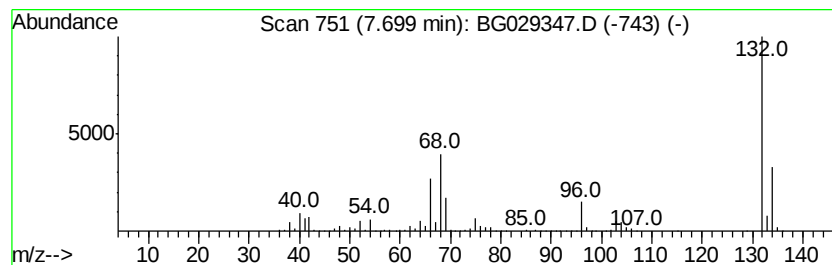
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Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	105.30 ng	1914170	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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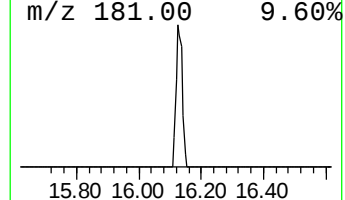
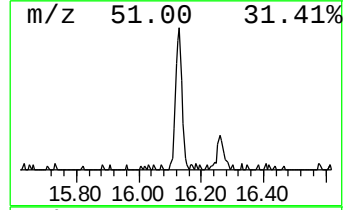
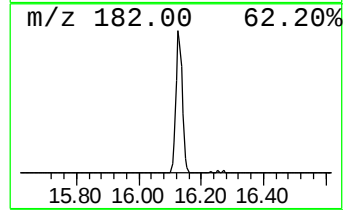
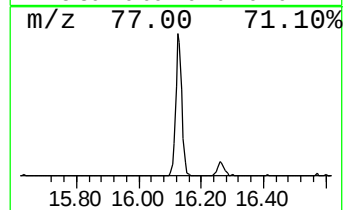
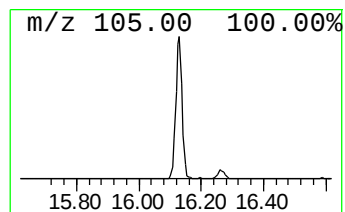
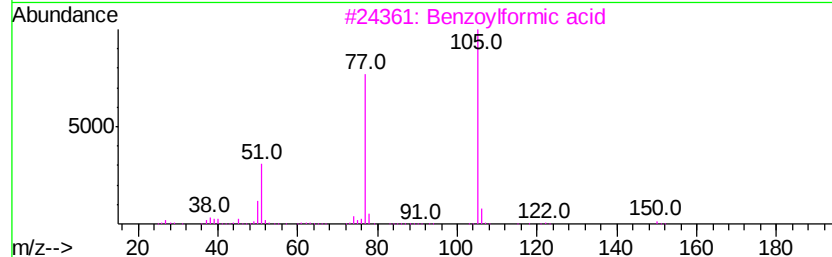
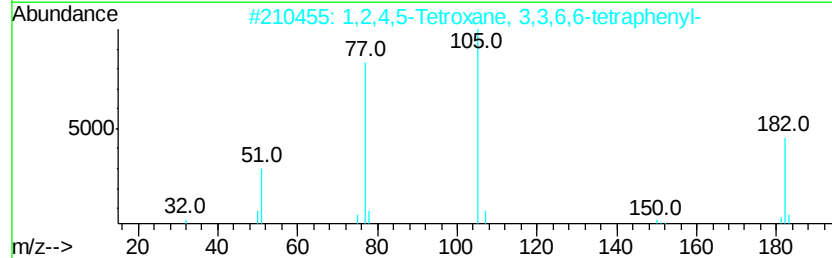
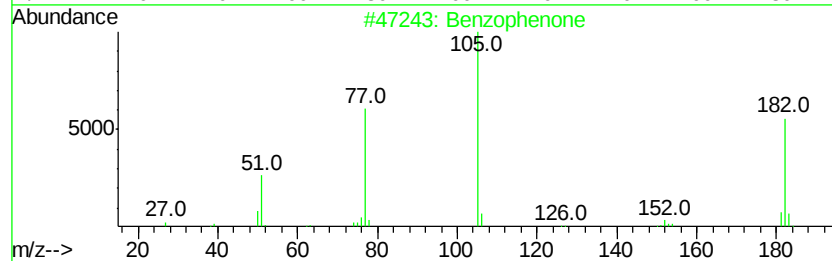
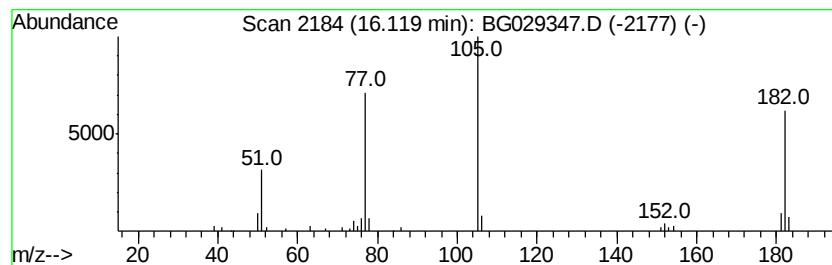
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Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	2.21 ng	93494	Acenaphthene-d10	14.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	97
2		1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3		Benzoylformic acid	150	C8H6O3	000611-73-4	49
4		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5		Benzilic acid	228	C14H12O3	000076-93-7	47



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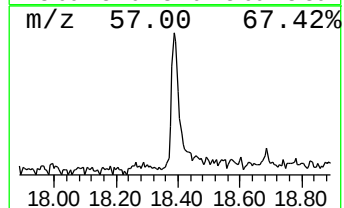
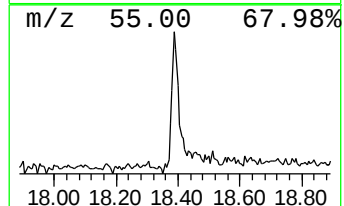
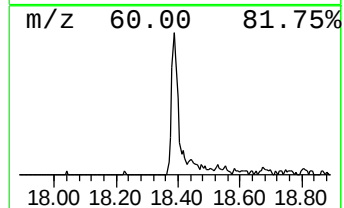
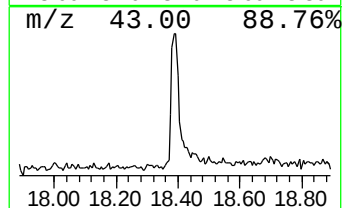
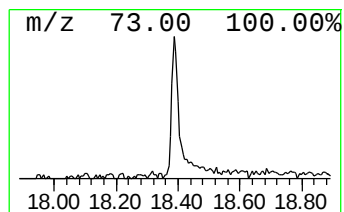
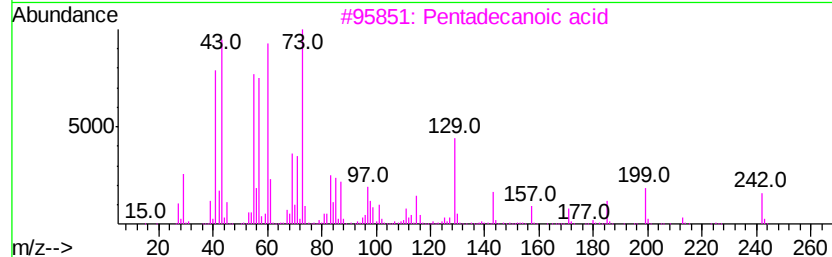
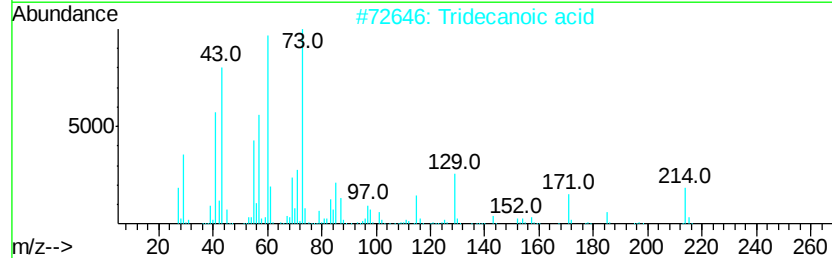
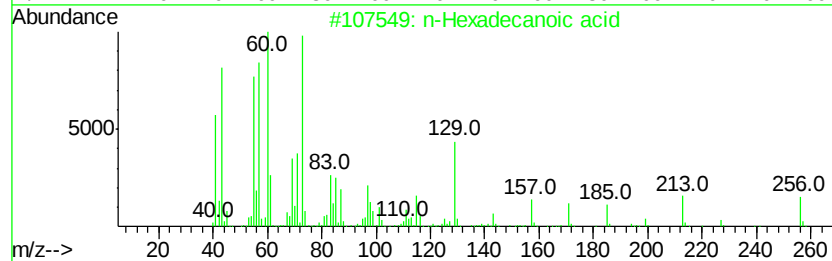
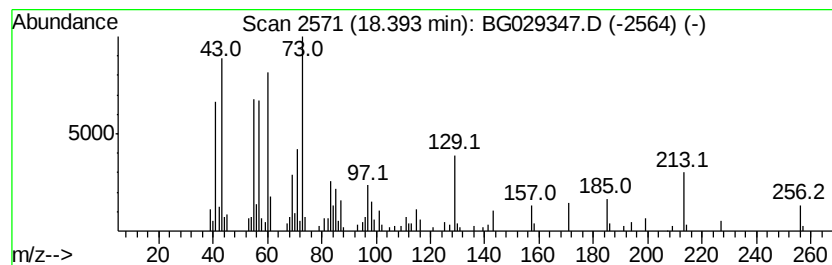
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.55 ng	152879	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



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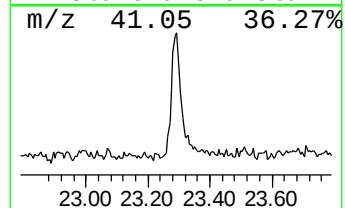
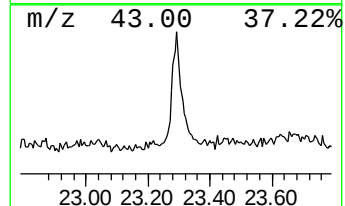
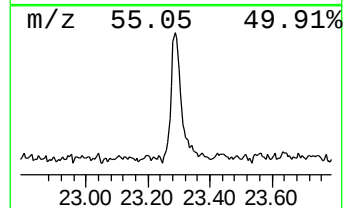
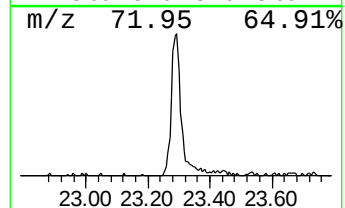
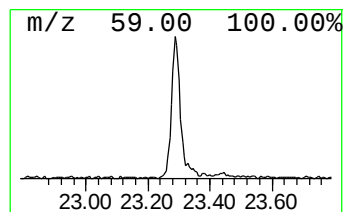
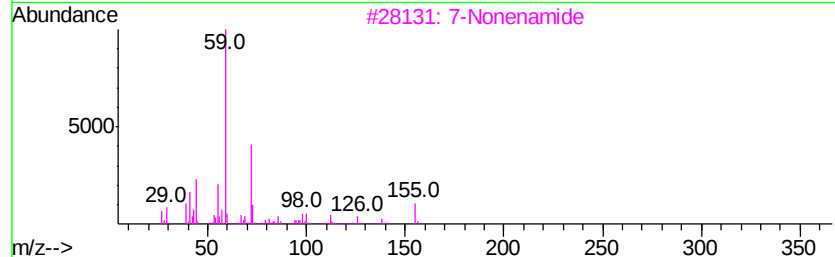
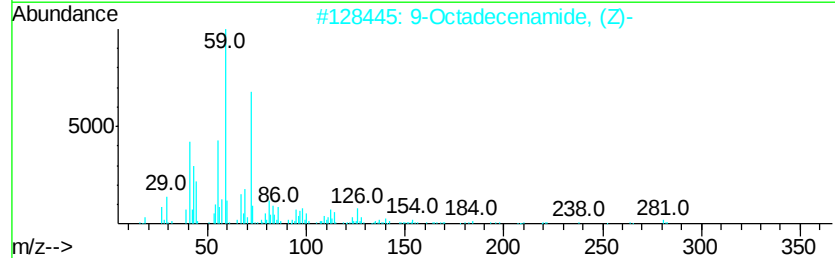
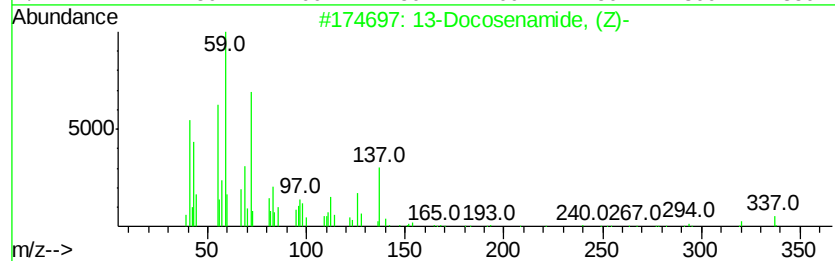
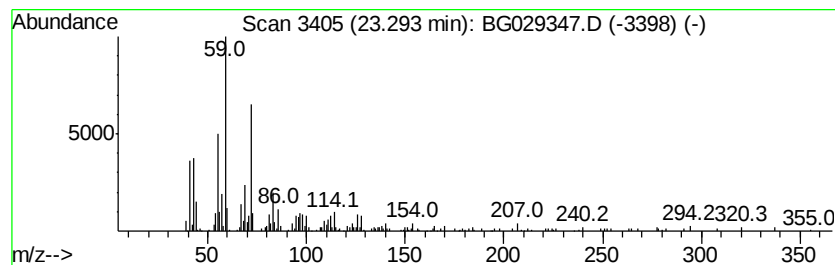
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Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	3.51 ng	262879	Chrysene-d12	21.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3		7-Nonenamide	155	C9H17NO	090949-53-4	72
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
5		Tetradecanamide	227	C14H29NO	000638-58-4	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	17.4	ng	315702	1	8.17	363552	20.0
unknown7.70	7.70	105.3	ng	1914170	1	8.17	363552	20.0
Benzophenone	16.12	2.2	ng	93494	3	14.79	846585	20.0
n-Hexadecanoic acid	18.39	2.5	ng	152879	4	17.52	1197900	20.0
13-Docosenamide, ...	23.29	3.5	ng	262879	5	21.79	1496530	20.0