

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101817\
 Data File : BG029350.D
 Acq On : 19 Oct 2017 3:09
 Operator : SJ/JU
 Sample : I5836-09
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ENV-125-11(20-30)

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	343	rVB	176271	267553	6.51%	1.159%
2	5.720	407	414	424	rBV	967422	1549927	37.74%	6.712%
3	7.318	678	686	698	rBV	982716	1764855	42.97%	7.642%
4	7.700	741	751	762	rBV	930671	1635591	39.83%	7.083%
5	8.164	824	830	838	rBV	206743	353712	8.61%	1.532%
6	8.493	878	886	894	rBV	666994	1175703	28.63%	5.091%
7	9.333	1021	1029	1037	rBV	530937	967461	23.56%	4.189%
8	10.984	1300	1310	1319	rBV	299398	531787	12.95%	2.303%
9	13.411	1715	1723	1732	rBV	1572642	2398168	58.40%	10.385%
10	14.227	1855	1862	1868	rBV	402103	598308	14.57%	2.591%
11	14.786	1950	1957	1965	rVB2	494374	803538	19.57%	3.480%
12	16.125	2177	2185	2194	rBV	63141	92798	2.26%	0.402%
13	16.266	2202	2209	2217	rBV	1537943	2340179	56.98%	10.134%
14	17.518	2416	2422	2430	rBV2	727194	1116694	27.19%	4.836%
15	18.387	2565	2570	2579	rBV2	54741	93880	2.29%	0.407%
16	20.109	2857	2863	2876	rBV	3092893	4106742	100.00%	17.783%
17	21.413	3081	3085	3093	rBV3	45471	84552	2.06%	0.366%
18	21.789	3142	3149	3162	rVB2	836283	1444799	35.18%	6.256%
19	23.287	3398	3404	3419	rVB	125853	273752	6.67%	1.185%
20	25.097	3701	3712	3726	rVB2	499811	1448244	35.27%	6.271%
21	26.296	3910	3916	3923	rVB8	16767	44859	1.09%	0.194%

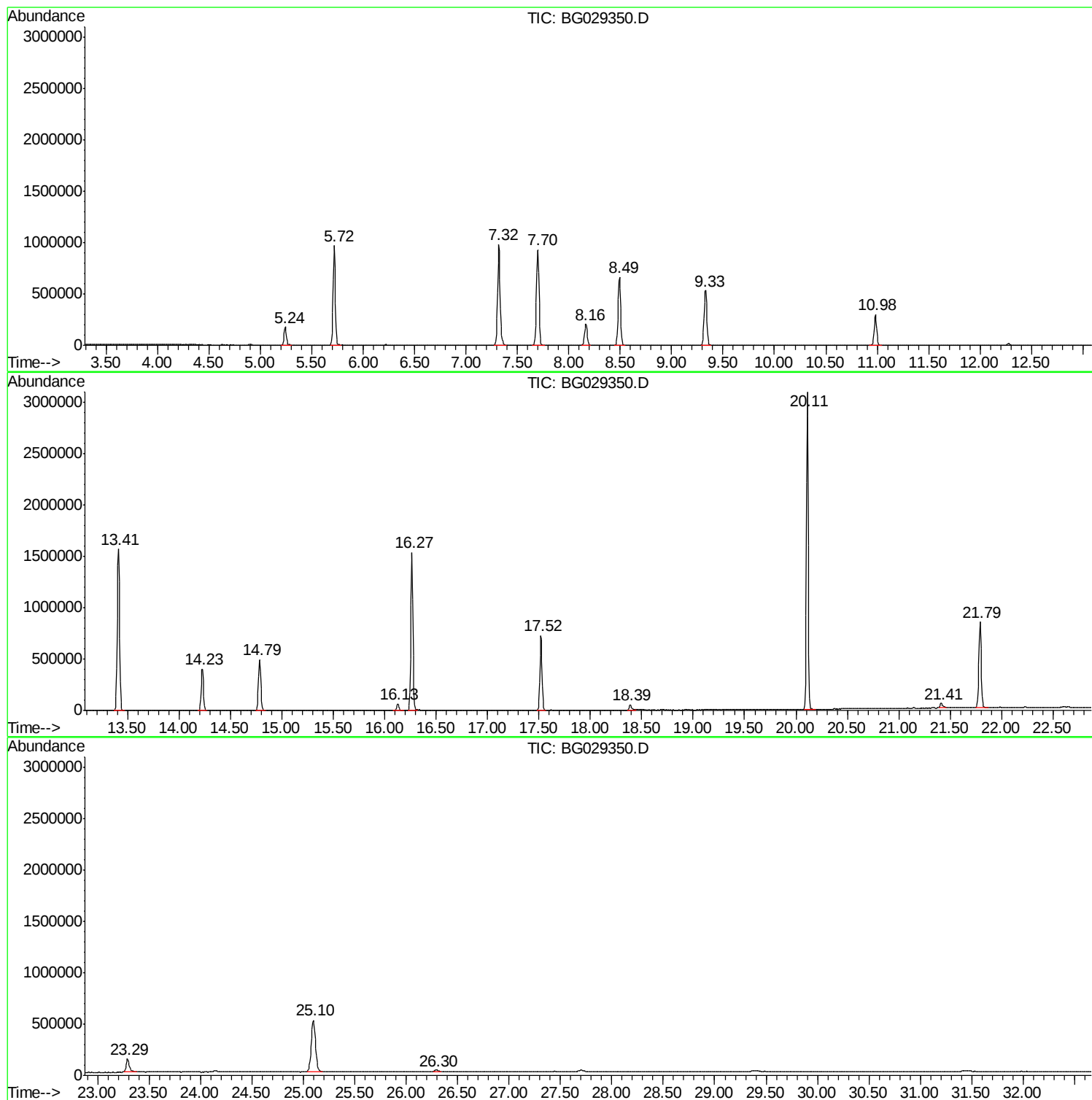
Sum of corrected areas: 23093102

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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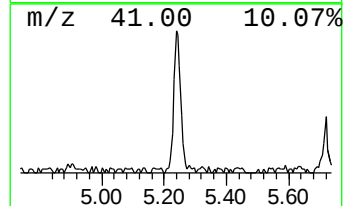
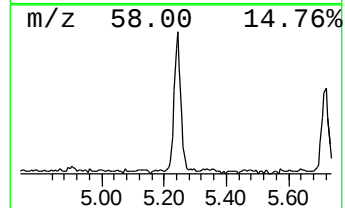
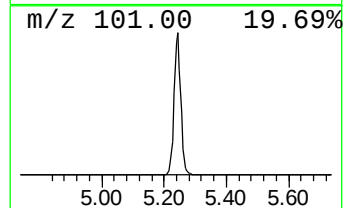
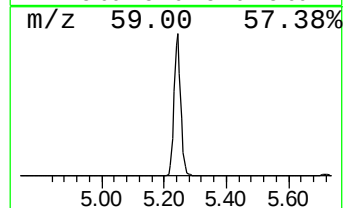
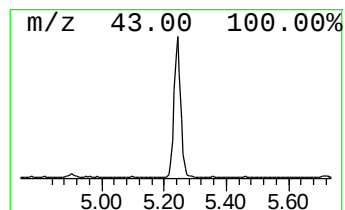
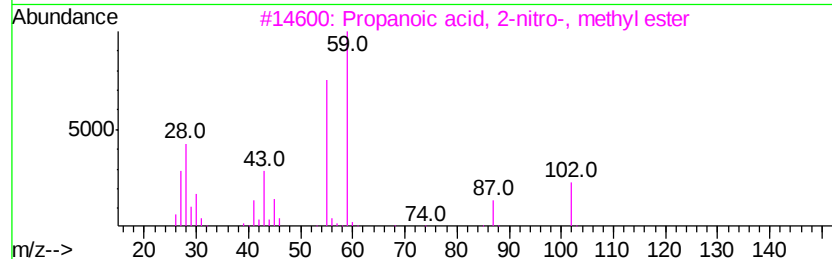
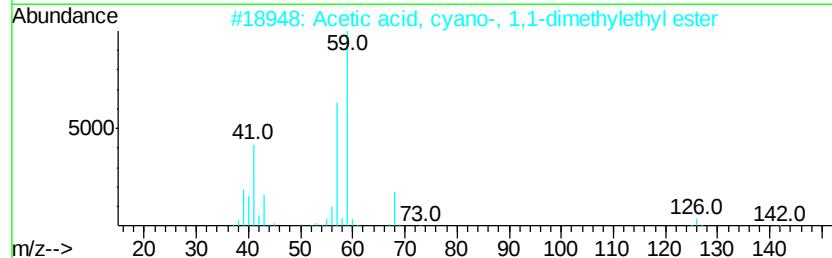
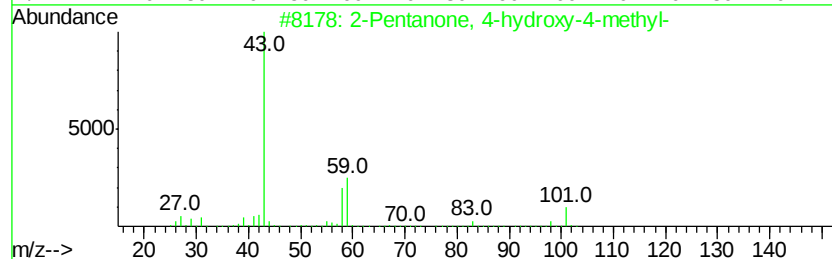
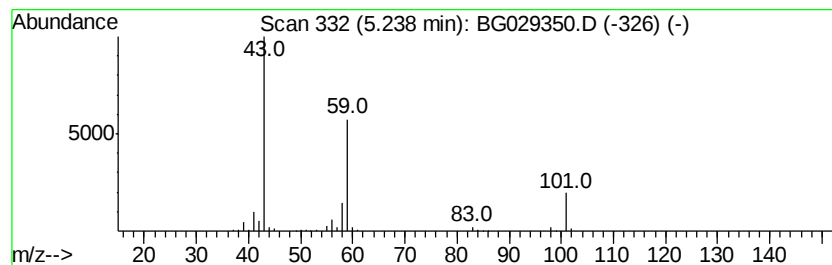
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	15.13 ng	267553	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
4		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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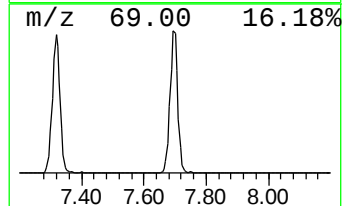
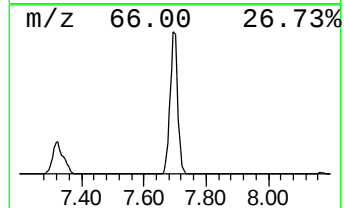
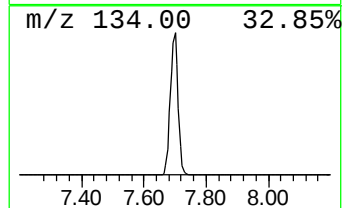
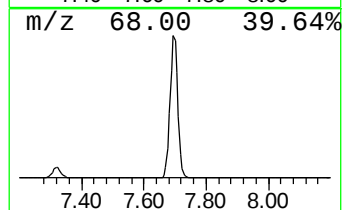
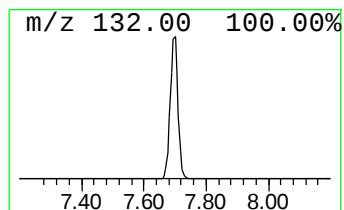
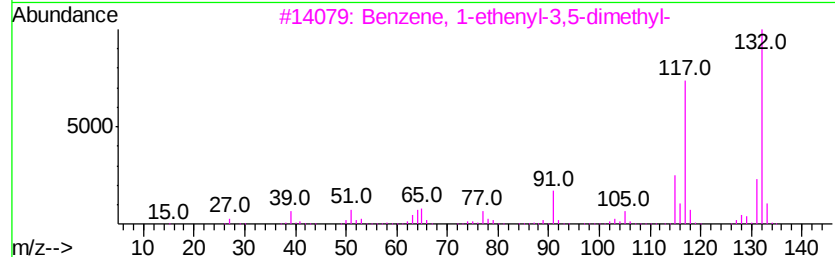
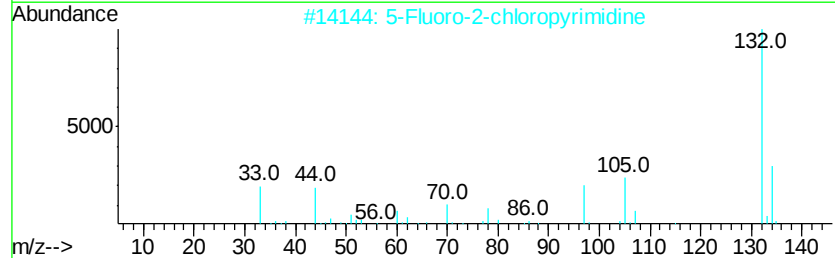
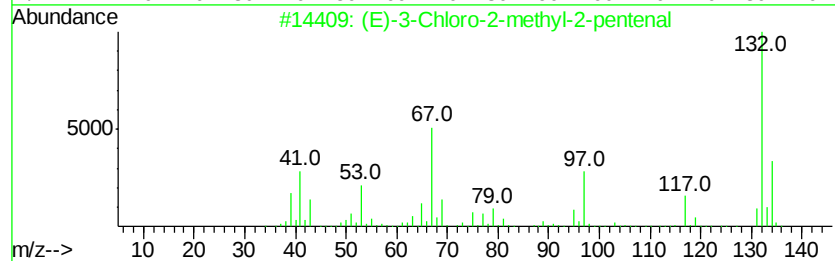
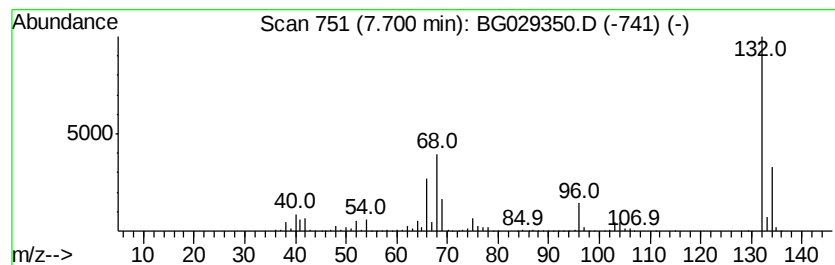
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Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	92.48 ng	1635590	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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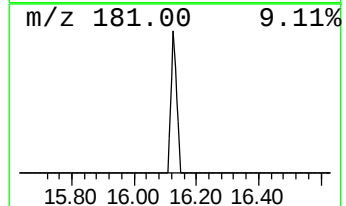
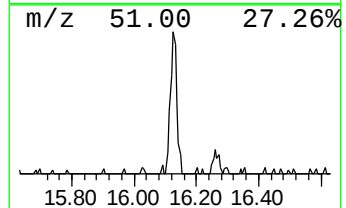
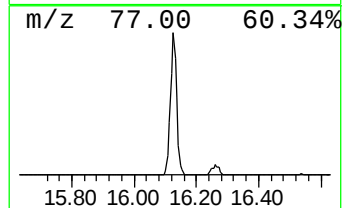
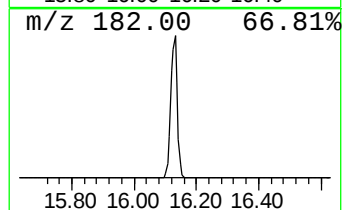
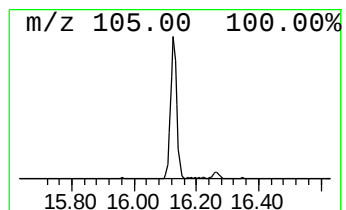
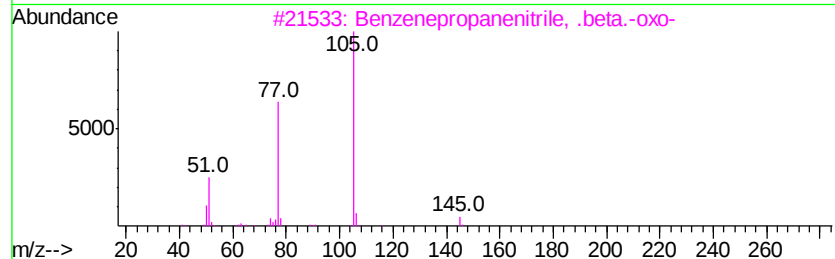
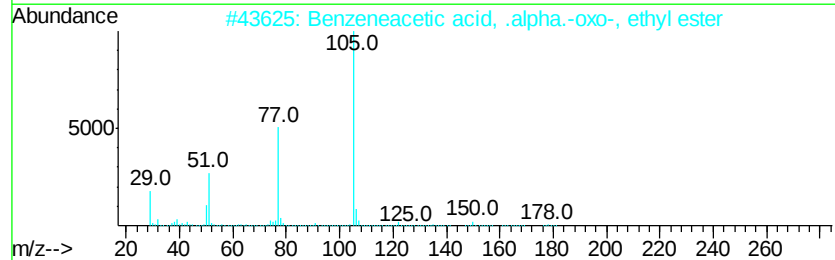
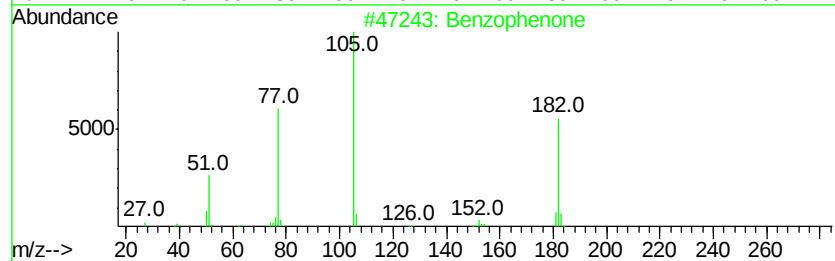
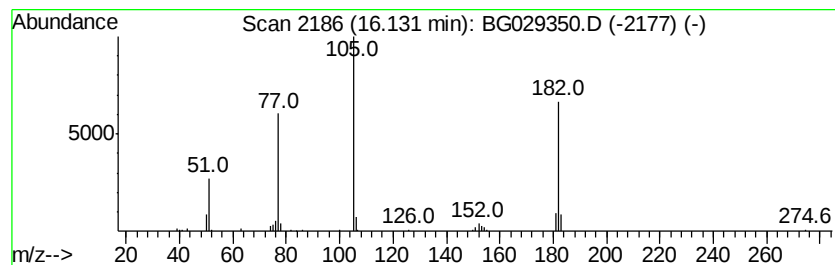
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Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.31 ng	92798	Acenaphthene-d10	14.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47
3	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
4	Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	47
5	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46



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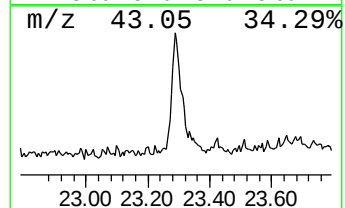
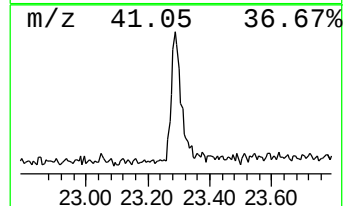
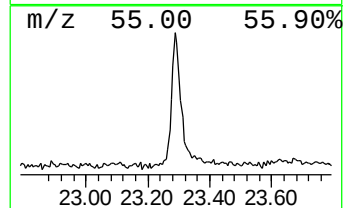
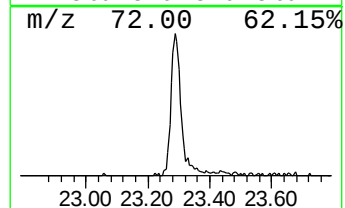
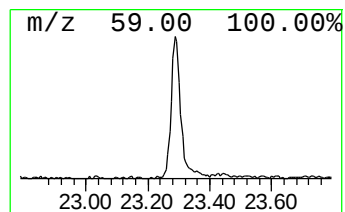
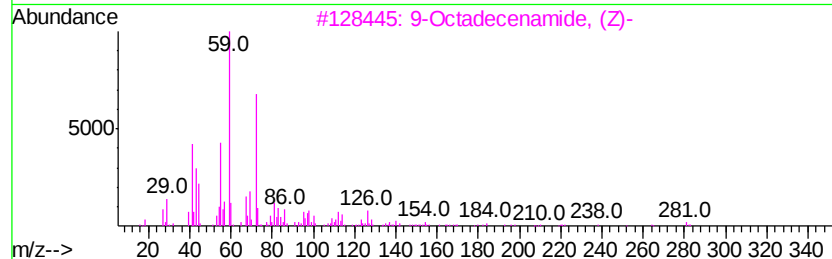
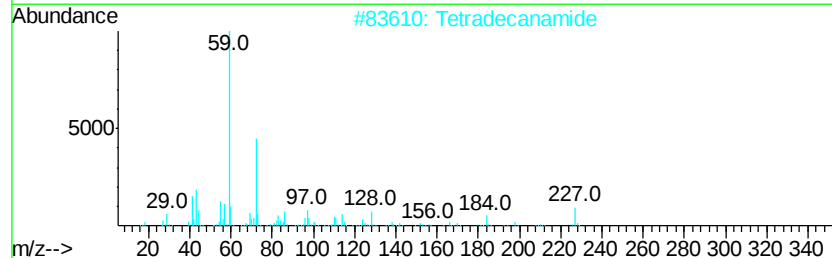
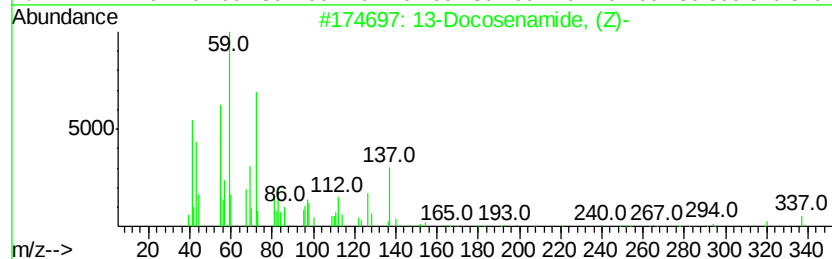
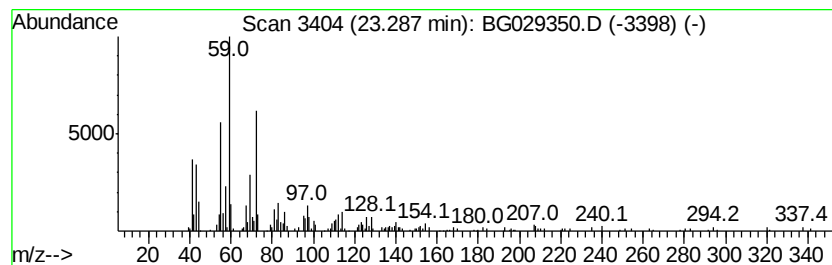
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Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	3.79 ng	273752	Chrysene-d12	21.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2		Tetradecanamide	227	C14H29NO	000638-58-4	90
3		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
4		Octadecanamide	283	C18H37NO	000124-26-5	80
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	15.1	ng	267553	1	8.16	353712	20.0
unknown7.70	7.70	92.5	ng	1635590	1	8.16	353712	20.0
Benzophenone	16.13	2.3	ng	92798	3	14.78	803538	20.0
13-Docosenamide, ...	23.29	3.8	ng	273752	5	21.79	1444800	20.0