

Data Path : Z:\HPCHEM1\BNA G\Data\BG032517\
 Data File : BG026426.D
 Acq On : 24 Mar 2017 22:27
 Operator : SJ/MA
 Sample : I2379-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-4

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-BG032017.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	5.145	344	350	361	rBV	189432	287454	3.61%	0.653%
2	5.615	423	430	448	rBV	1840946	3024961	38.01%	6.870%
3	7.207	693	701	717	rBV	1755169	3013174	37.86%	6.843%
4	7.577	756	764	778	rBV	1931685	3309123	41.58%	7.515%
5	8.041	836	843	855	rBV	457202	790628	9.93%	1.796%
6	8.365	891	898	907	rBV	1524464	2645250	33.24%	6.008%
7	9.199	1030	1040	1053	rBV	1041453	1859733	23.37%	4.224%
8	10.844	1311	1320	1333	rBV	628952	1146005	14.40%	2.603%
9	13.276	1726	1734	1747	rBV	3263495	4986340	62.65%	11.324%
10	14.099	1863	1874	1883	rBV	193949	317124	3.98%	0.720%
11	14.610	1954	1961	1963	rBV	205793	288998	3.63%	0.656%
12	14.651	1963	1968	1977	rVB2	969545	1579976	19.85%	3.588%
13	16.126	2210	2219	2240	rBV	2465016	3940835	49.52%	8.950%
14	16.338	2250	2255	2258	rBV	70776	98697	1.24%	0.224%
15	17.383	2426	2433	2443	rBV	1364877	2091003	26.27%	4.749%
16	18.259	2576	2582	2590	rBV	248857	363303	4.56%	0.825%
17	19.522	2793	2797	2803	rBV2	59688	89278	1.12%	0.203%
18	19.980	2869	2875	2883	rBV	5991556	7958739	100.00%	18.075%
19	21.085	3058	3063	3072	rVB	288338	394495	4.96%	0.896%
20	21.267	3090	3094	3104	rBV3	107198	236108	2.97%	0.536%
21	21.625	3148	3155	3165	rBV	1744418	2821066	35.45%	6.407%
22	24.804	3685	3696	3711	rBV2	981649	2789355	35.05%	6.335%

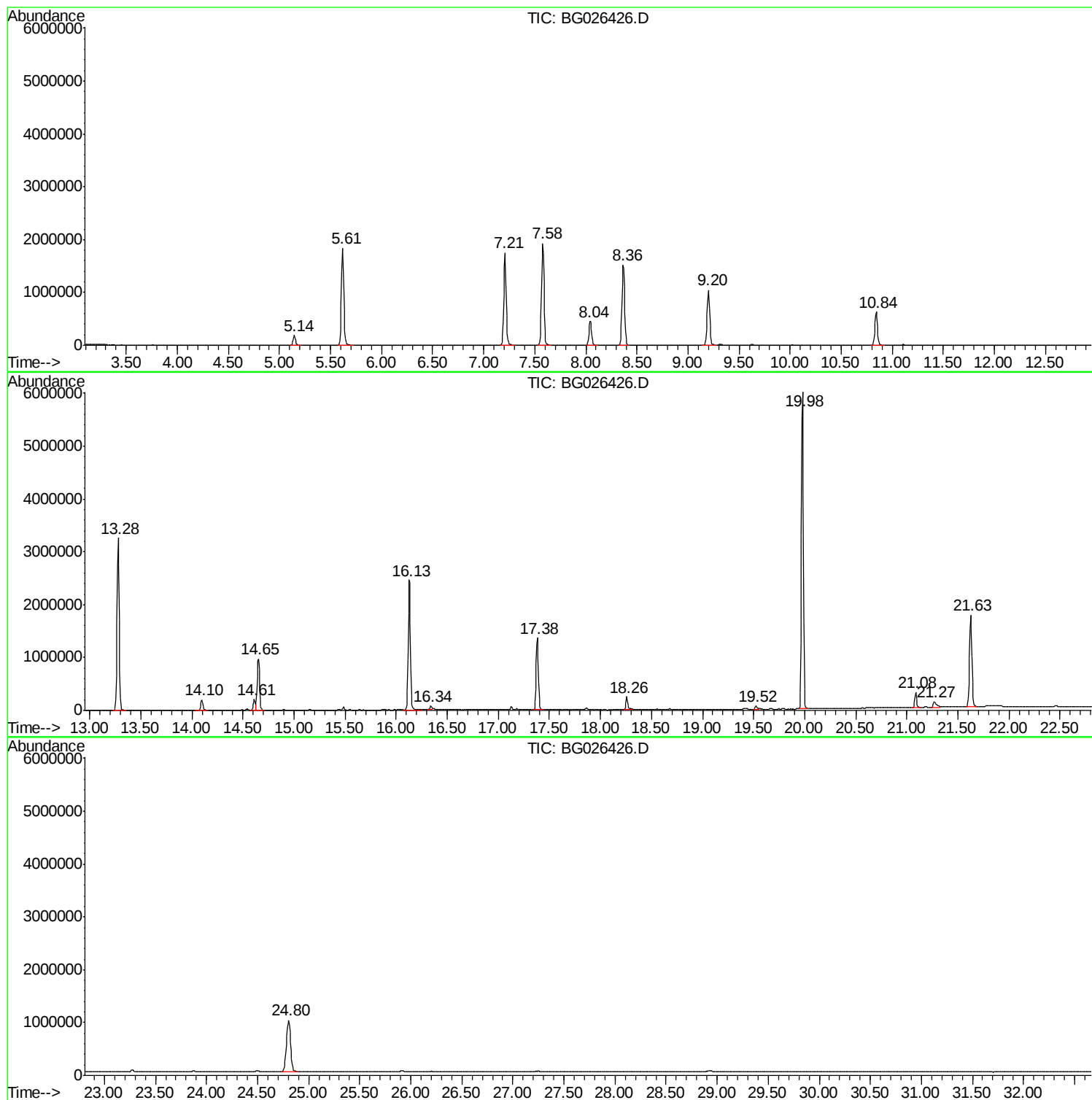
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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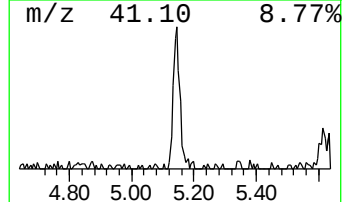
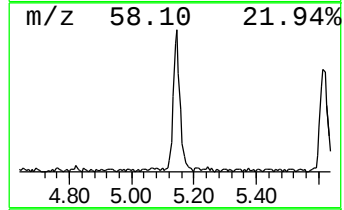
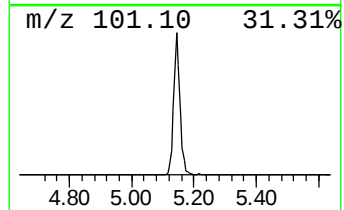
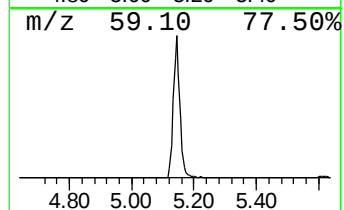
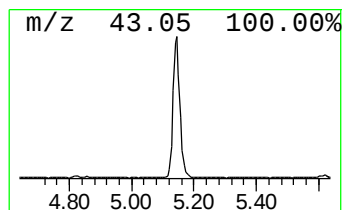
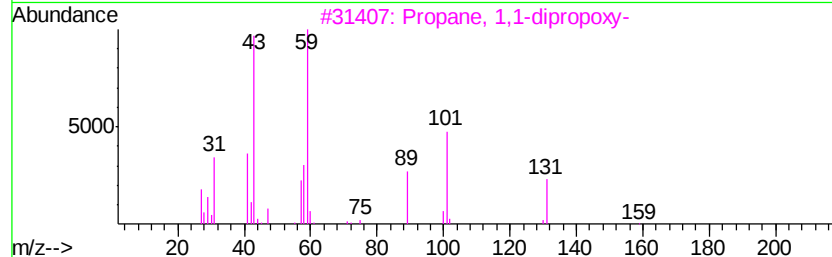
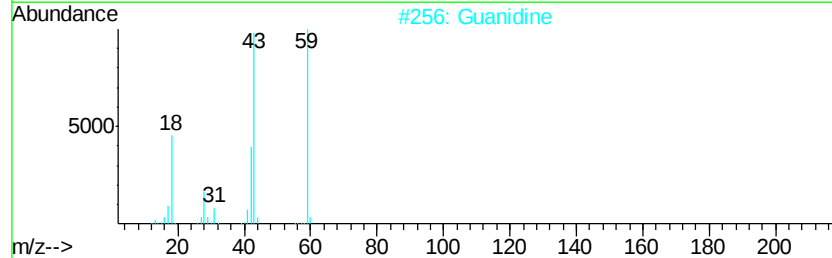
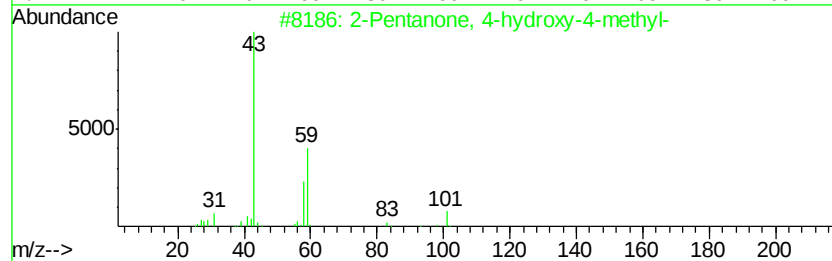
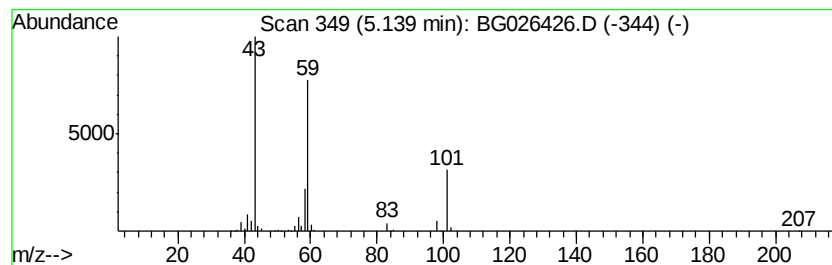
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	7.27 ng	287454	1,4-Dichlorobenzene-d4	8.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Guanidine	59	CH5N3	000113-00-8	47
3			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	40
4			Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	36
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28



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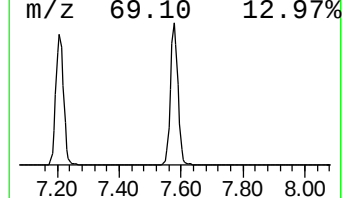
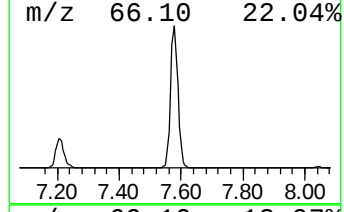
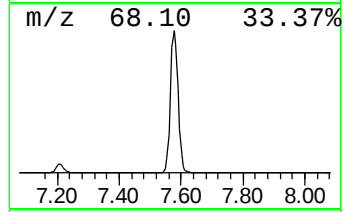
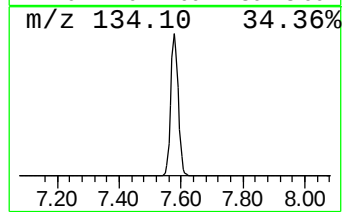
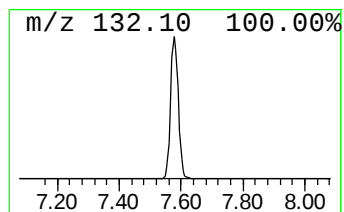
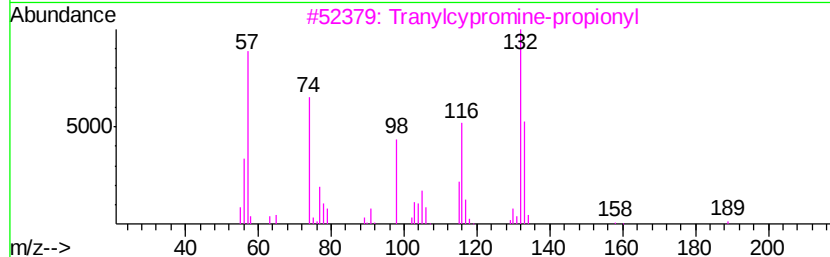
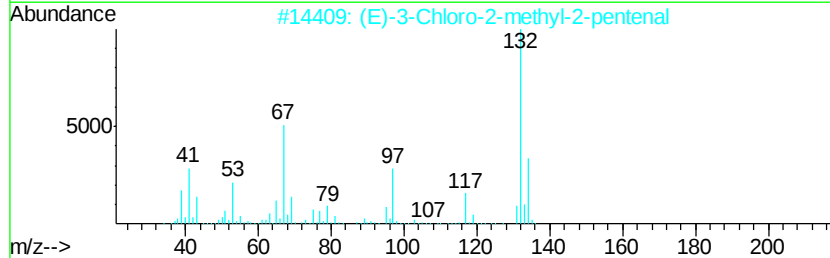
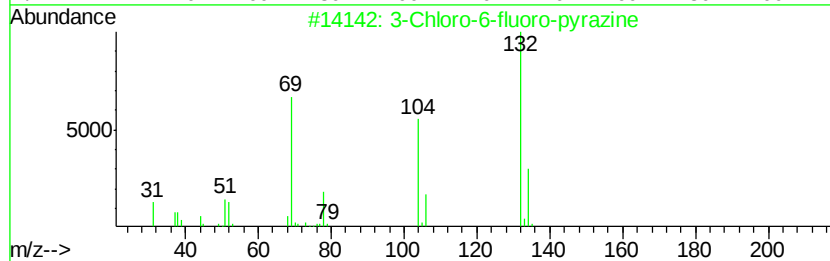
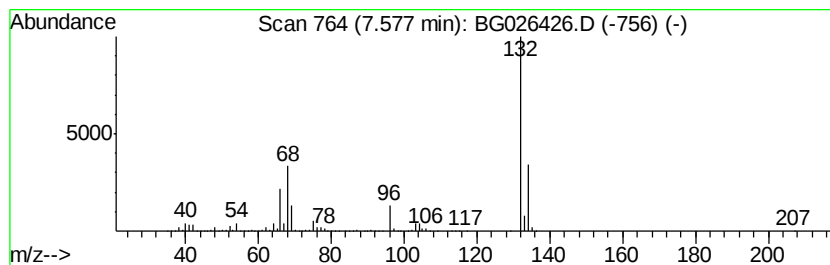
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Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	83.71 ng	3309120	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypramine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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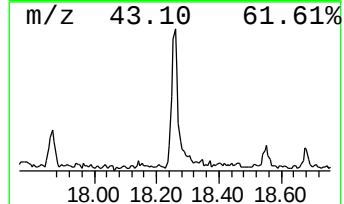
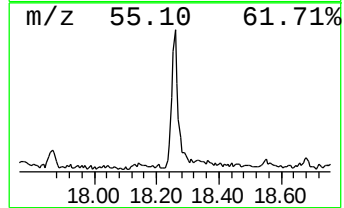
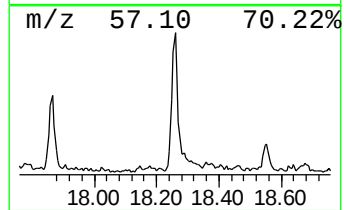
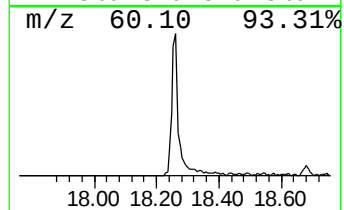
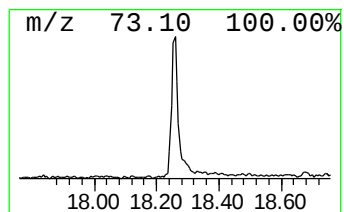
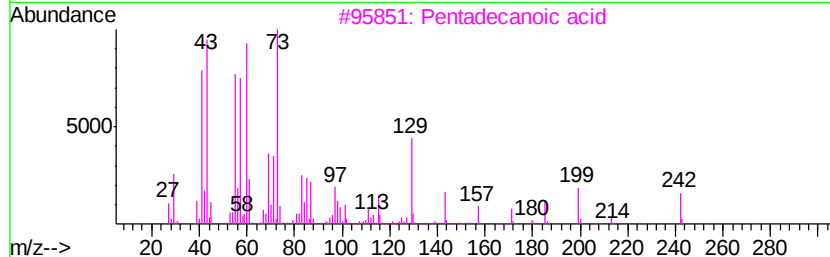
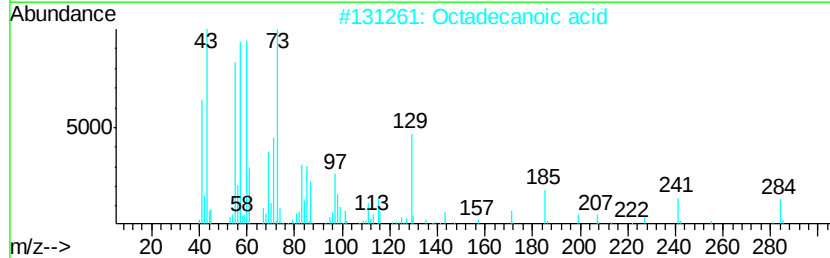
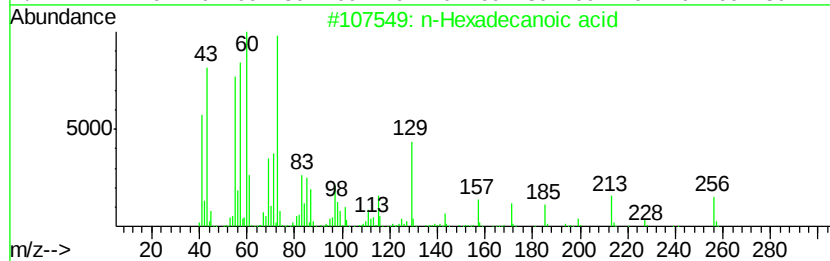
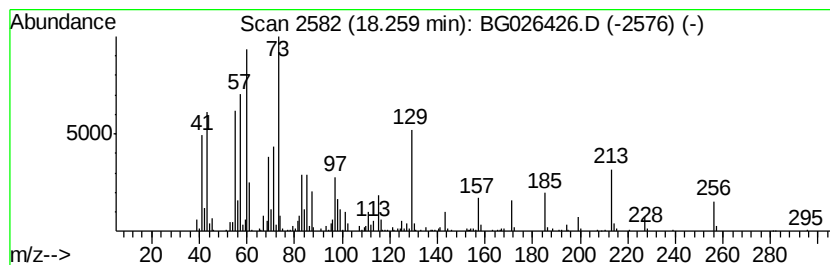
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.26	3.47 ng	363303	Phenanthrene-d10	17.38		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Octadecanoic acid	284	C18H36O2	000057-11-4	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Tridecanoic acid	214	C13H26O2	000638-53-9	70



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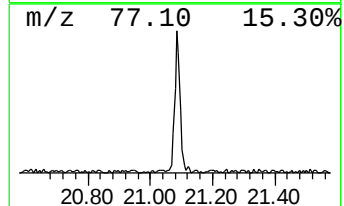
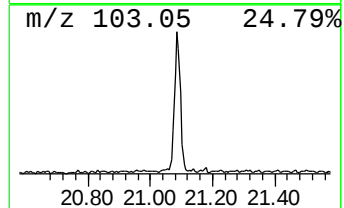
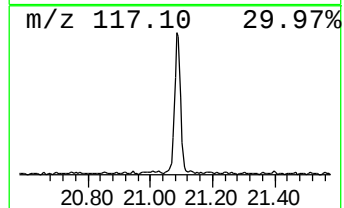
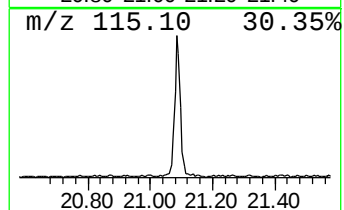
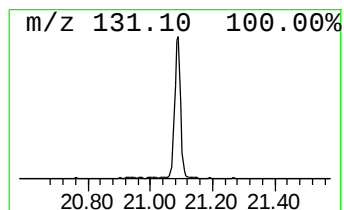
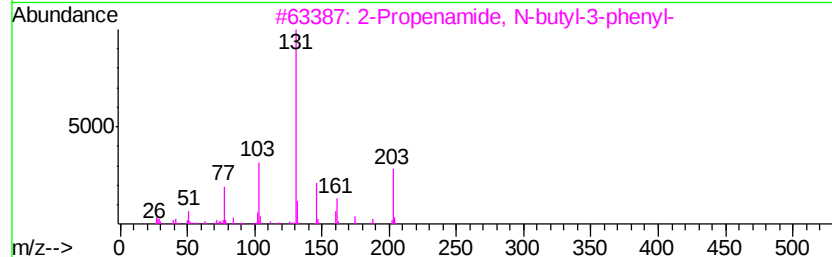
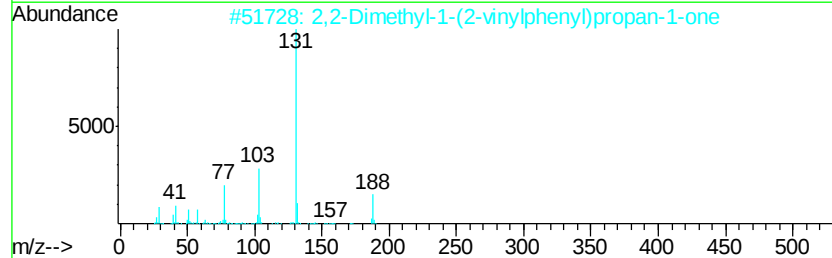
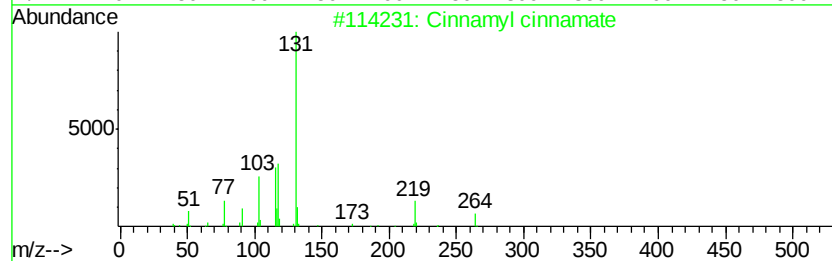
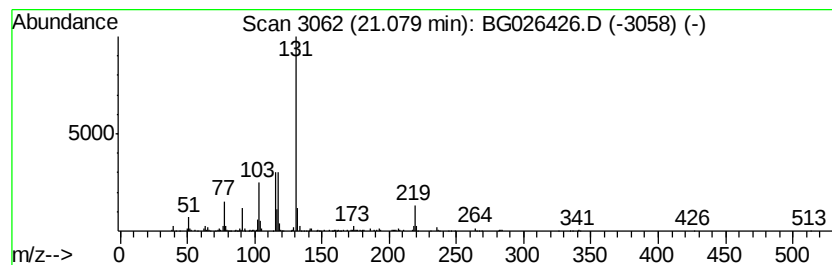
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Peak Number 5 Cinnamyl cinnamate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.08	2.80 ng	394495	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2		2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	49
3		2-Propenamide, N-butyl-3-phenyl-	203	C13H17NO	006299-56-5	47
4		1H-Indole, 1-methyl-	131	C9H9N	000603-76-9	47
5		1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	7.3	ng	287454	1	8.04	790628	20.0
unknown7.58	7.58	83.7	ng	3309120	1	8.04	790628	20.0
n-Hexadecanoic acid	18.26	3.5	ng	363303	4	17.38	2091000	20.0
Cinnamyl cinnamate	21.08	2.8	ng	394495	5	21.63	2821070	20.0