

Data Path : Z:\HPCHEM1\BNA G\DATA\BG063017\
 Data File : BG027767.D
 Acq On : 30 Jun 2017 23:46
 Operator : SJ/JU
 Sample : I3908-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 G-60-1.5-3

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-BG062817.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	5.609	286	293	302	rBV	88208	143387	5.65%	0.929%
2	6.056	362	369	382	rBV	657212	1104517	43.52%	7.156%
3	7.619	627	635	648	rBV	671508	1226684	48.34%	7.948%
4	8.012	693	702	713	rBV	647110	1160174	45.72%	7.517%
5	8.477	774	781	794	rVB	126235	234908	9.26%	1.522%
6	8.806	830	837	847	rVB	423408	790330	31.14%	5.121%
7	9.640	969	979	989	rBV	384541	726795	28.64%	4.709%
8	11.297	1254	1261	1268	rBV	196740	374951	14.77%	2.429%
9	13.694	1659	1669	1681	rBV	1016425	1614256	63.61%	10.459%
10	14.499	1800	1806	1814	rBV	184534	284822	11.22%	1.845%
11	15.069	1896	1903	1911	rVB2	325797	547852	21.59%	3.550%
12	15.868	2034	2039	2044	rVB	23587	32489	1.28%	0.210%
13	16.555	2148	2156	2165	rBV	991156	1555670	61.30%	10.079%
14	16.726	2180	2185	2195	rBV2	26750	48586	1.91%	0.315%
15	17.525	2316	2321	2326	rBV	18405	26211	1.03%	0.170%
16	17.819	2365	2371	2377	rBV	458738	727651	28.67%	4.714%
17	18.153	2422	2428	2437	rBV2	25731	48791	1.92%	0.316%
18	18.665	2510	2515	2523	rBV3	37536	73584	2.90%	0.477%
19	19.499	2653	2657	2664	rBV	94308	146703	5.78%	0.950%
20	19.587	2669	2672	2676	rVB2	58816	70828	2.79%	0.459%
21	19.916	2723	2728	2734	rBV5	21868	38930	1.53%	0.252%
22	20.392	2803	2809	2820	rVB	1835081	2537835	100.00%	16.443%
23	21.015	2911	2915	2919	rBV	40226	53002	2.09%	0.343%
24	21.068	2919	2924	2933	rVB	130175	192466	7.58%	1.247%
25	21.737	3033	3038	3051	rVB9	21063	49189	1.94%	0.319%
26	22.008	3079	3084	3090	rBV	21910	35945	1.42%	0.233%
27	22.178	3104	3113	3127	rBV	434751	801975	31.60%	5.196%
28	25.792	3712	3728	3743	rBV2	232160	785940	30.97%	5.092%

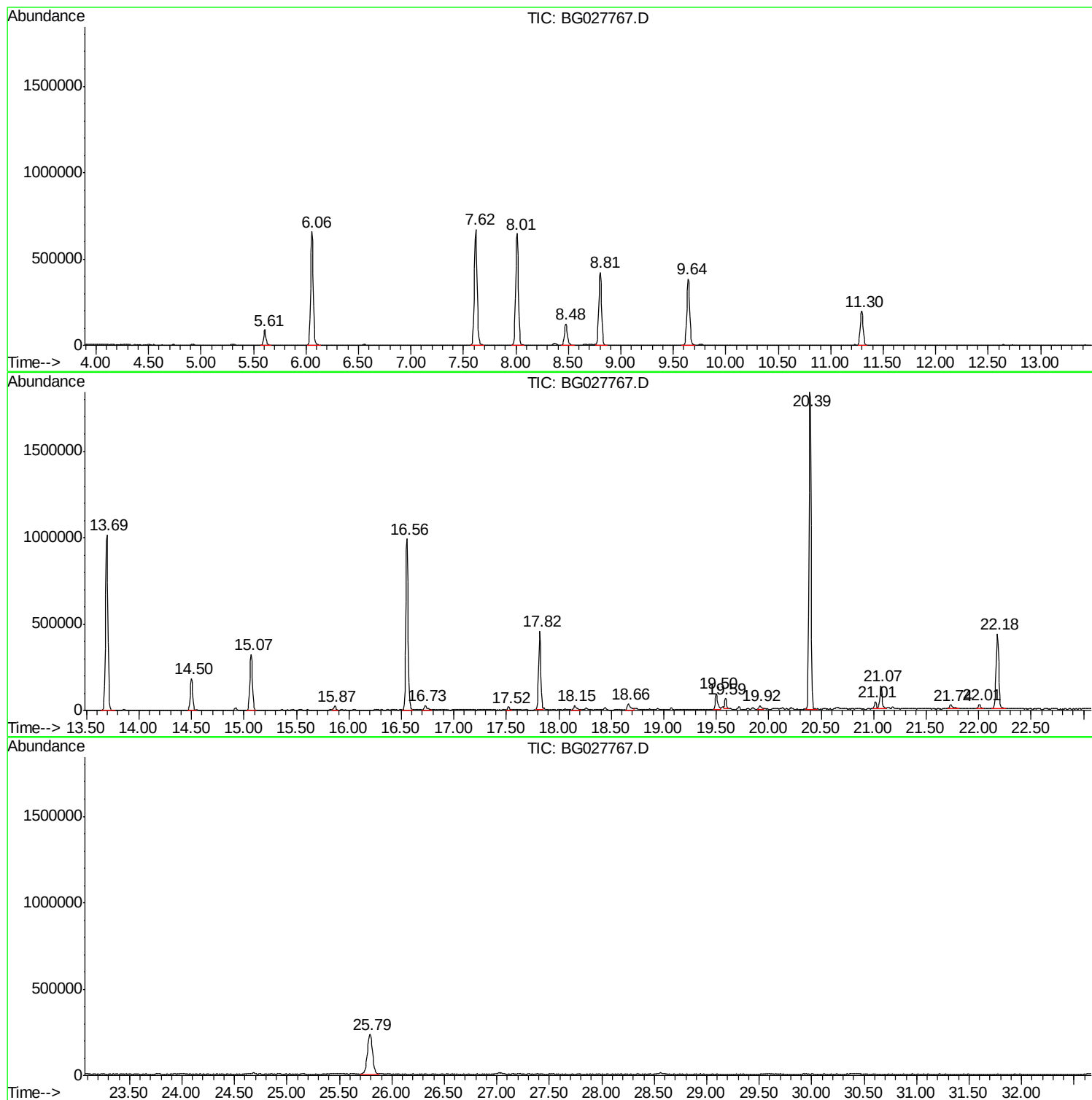
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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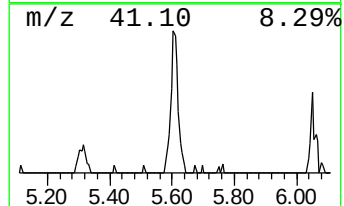
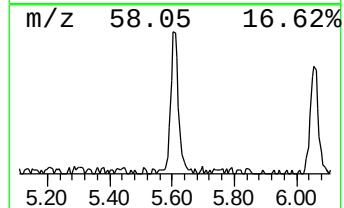
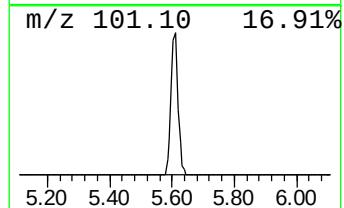
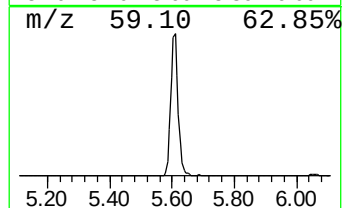
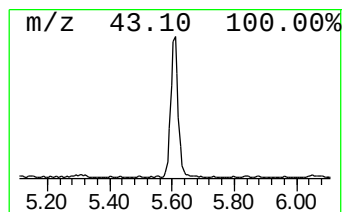
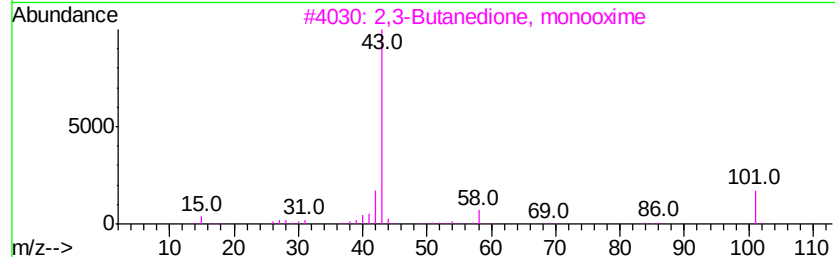
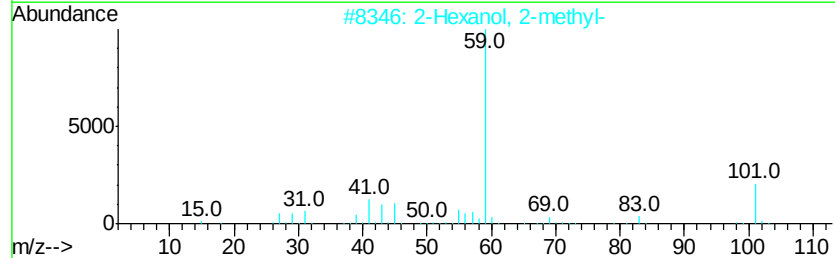
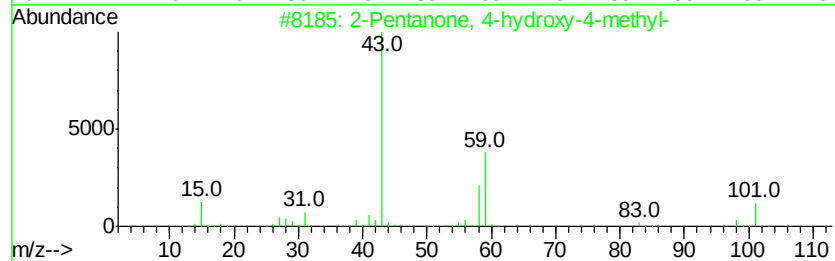
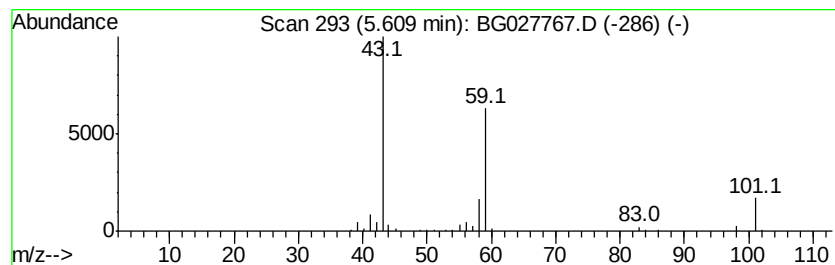
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG062817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.61	12.21 ng	143387	1,4-Dichlorobenzene-d4	8.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Guanidine	59	CH5N3	000113-00-8	9
5		2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9



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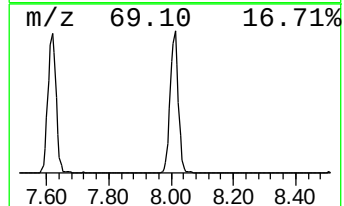
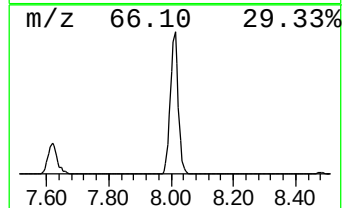
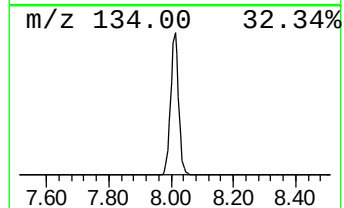
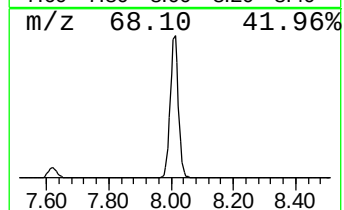
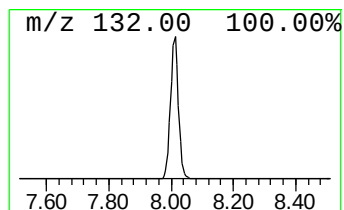
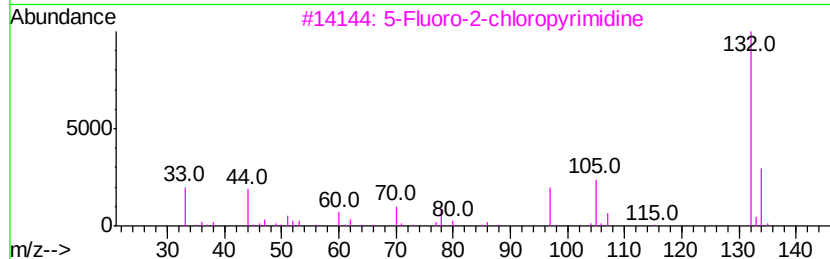
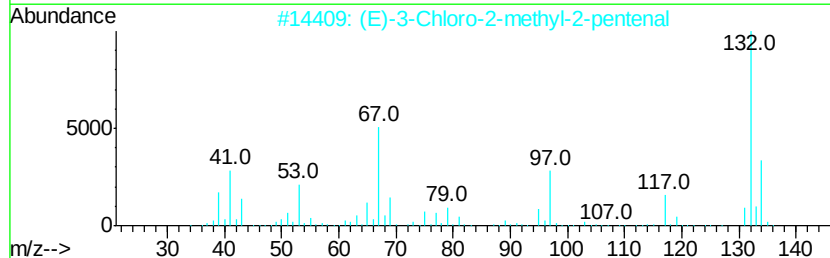
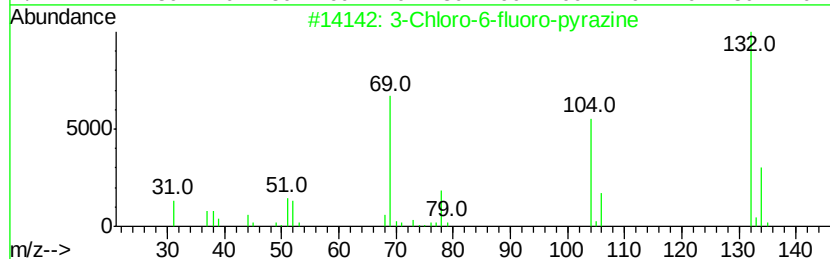
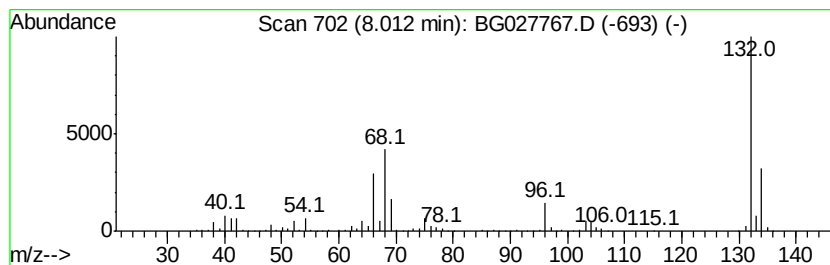
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Peak Number 2 unknown8.01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	98.78 ng	1160170	1,4-Dichlorobenzene-d4	8.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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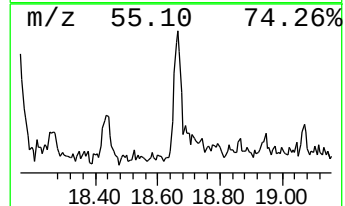
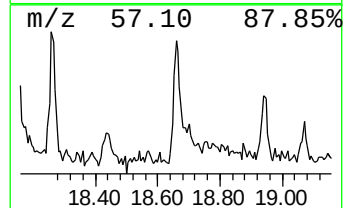
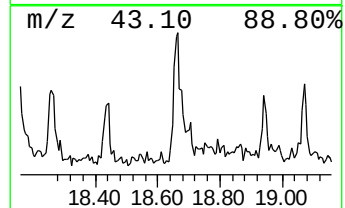
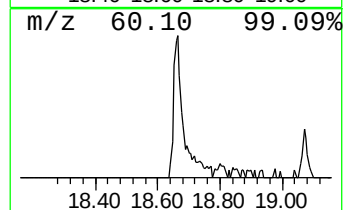
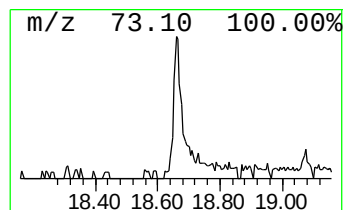
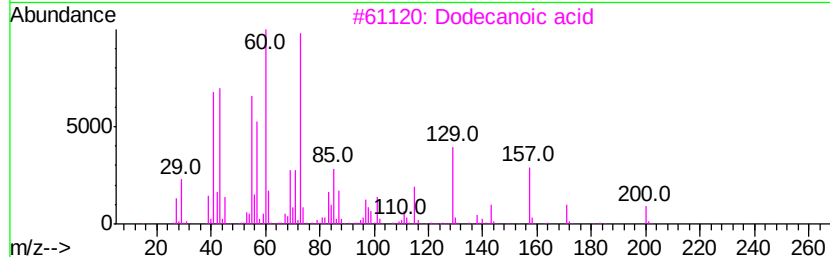
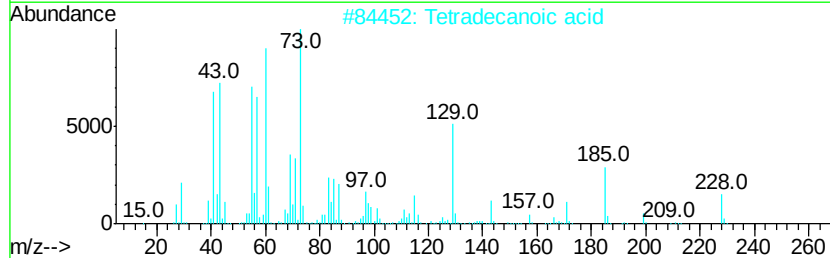
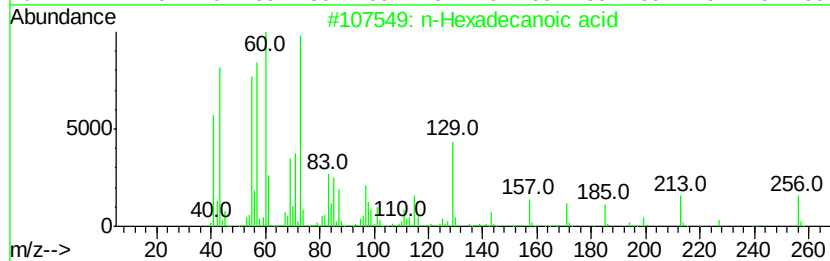
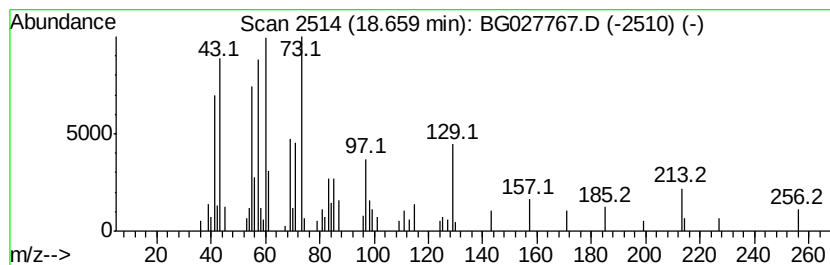
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.66	2.02 ng	73584	Phenanthrene-d10	17.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64



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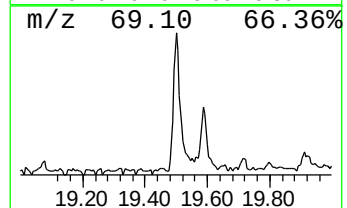
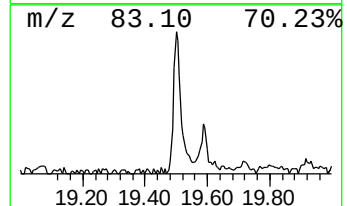
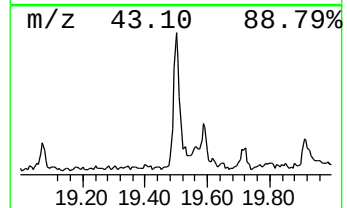
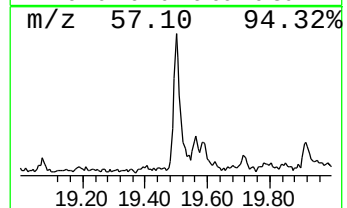
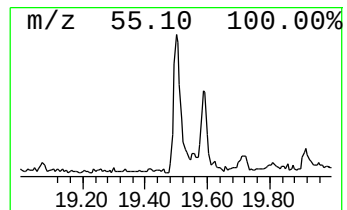
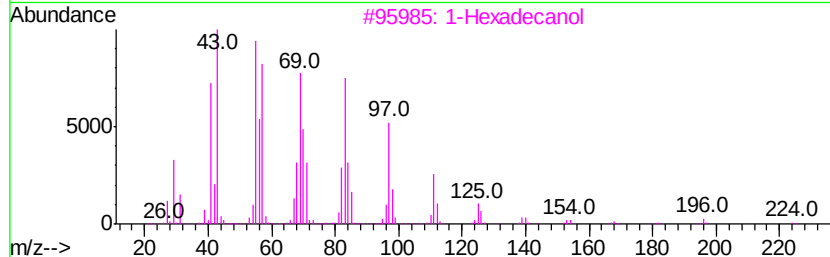
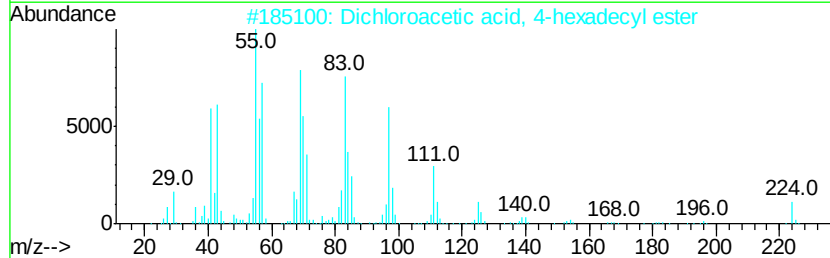
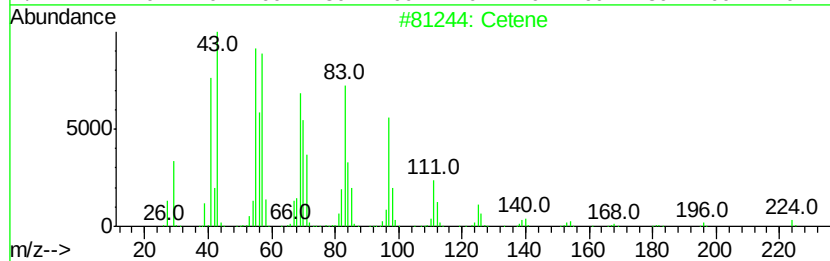
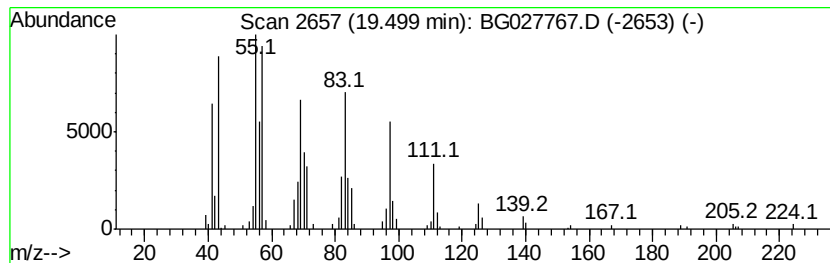
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Peak Number 5 Cetene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.50	4.03 ng	146703	Phenanthrene-d10	17.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	96
2	Dichloroacetic acid, 4-hexadecyl...	352	C18H34Cl2O2	1000282-98-1	94
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91



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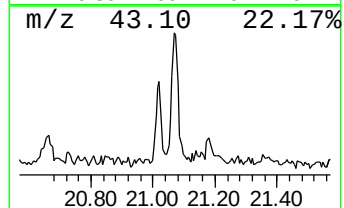
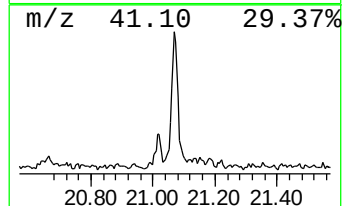
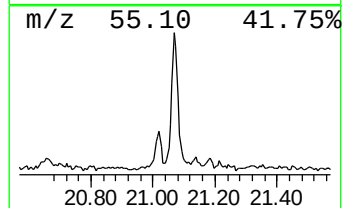
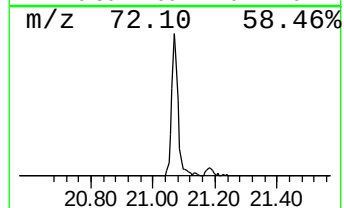
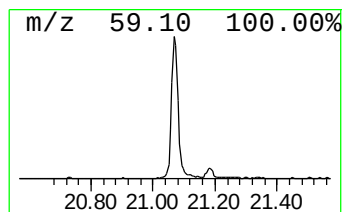
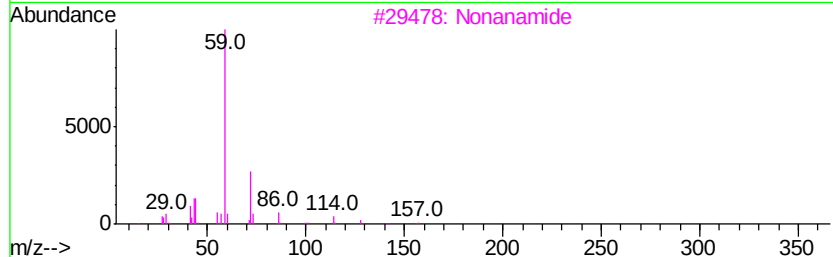
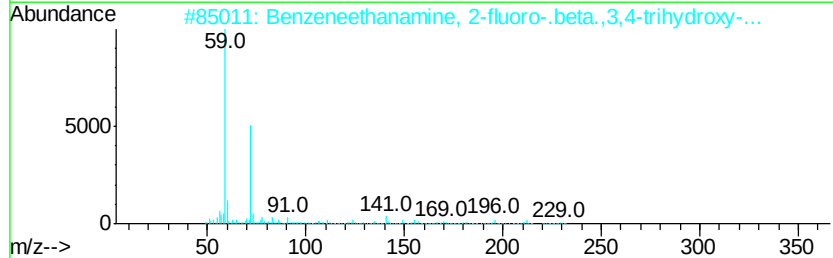
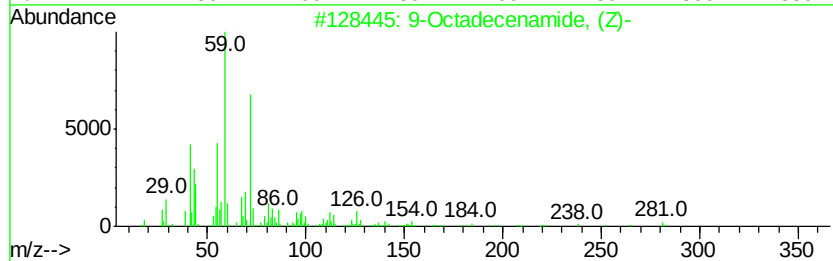
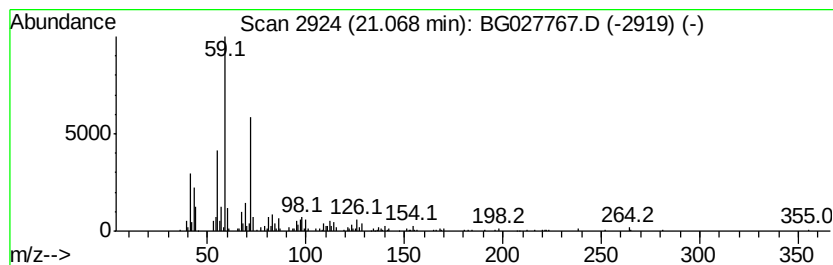
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.07	4.80 ng	192466	Chrysene-d12	22.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	72
3		Nonanamide	157	C9H19NO	001120-07-6	59
4		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
5		Dodecanamide	199	C12H25NO	001120-16-7	50



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TIC Library : C:\Database\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.61	12.2	ng	143387	1	8.48	234908	20.0
unknown8.01	8.01	98.8	ng	1160170	1	8.48	234908	20.0
n-Hexadecanoic acid	18.66	2.0	ng	73584	4	17.82	727651	20.0
Cetene	19.50	4.0	ng	146703	4	17.82	727651	20.0
9-Octadecenamide,...	21.07	4.8	ng	192466	5	22.18	801975	20.0