

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121518\
 Data File : BG038634.D
 Acq On : 16 Dec 2018 10:47
 Operator : JU/SJ
 Sample : J6397-04
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EB11 12-14

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-BG121218.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	5.143	345	350	358	rBV	26243	42527	2.35%	0.443%
2	5.608	422	429	440	rVB	445573	723152	39.92%	7.540%
3	7.212	694	702	715	rBV	464095	875197	48.32%	9.125%
4	7.588	758	766	777	rBV	426239	765076	42.24%	7.977%
5	8.058	840	846	855	rBV	81970	141250	7.80%	1.473%
6	8.381	893	901	910	rBV	323328	585100	32.30%	6.100%
7	9.239	1039	1047	1056	rBV	275156	523507	28.90%	5.458%
8	10.878	1318	1326	1334	rBV	100749	194532	10.74%	2.028%
9	13.316	1734	1741	1753	rBV	761805	1218579	67.27%	12.705%
10	14.139	1875	1881	1887	rBV2	39048	62218	3.43%	0.649%
11	14.697	1969	1976	1987	rVB2	169392	288002	15.90%	3.003%
12	16.183	2222	2229	2243	rBV	609031	947999	52.34%	9.884%
13	17.441	2437	2443	2453	rBV2	238589	362846	20.03%	3.783%
14	18.304	2585	2590	2606	rBV2	33047	58689	3.24%	0.612%
15	20.044	2880	2886	2892	rBV	1358377	1811401	100.00%	18.886%
16	21.319	3098	3103	3117	rBV	56612	106322	5.87%	1.109%
17	21.718	3163	3171	3179	rBV2	230078	395353	21.83%	4.122%
18	23.175	3411	3419	3427	rBV9	9026	18146	1.00%	0.189%
19	23.363	3445	3451	3457	rBV3	11846	23447	1.29%	0.244%
20	23.986	3549	3557	3563	rBV7	7726	19107	1.05%	0.199%
21	25.020	3722	3733	3743	rVB2	134401	388396	21.44%	4.049%
22	26.260	3934	3944	3946	rBV10	14771	40505	2.24%	0.422%

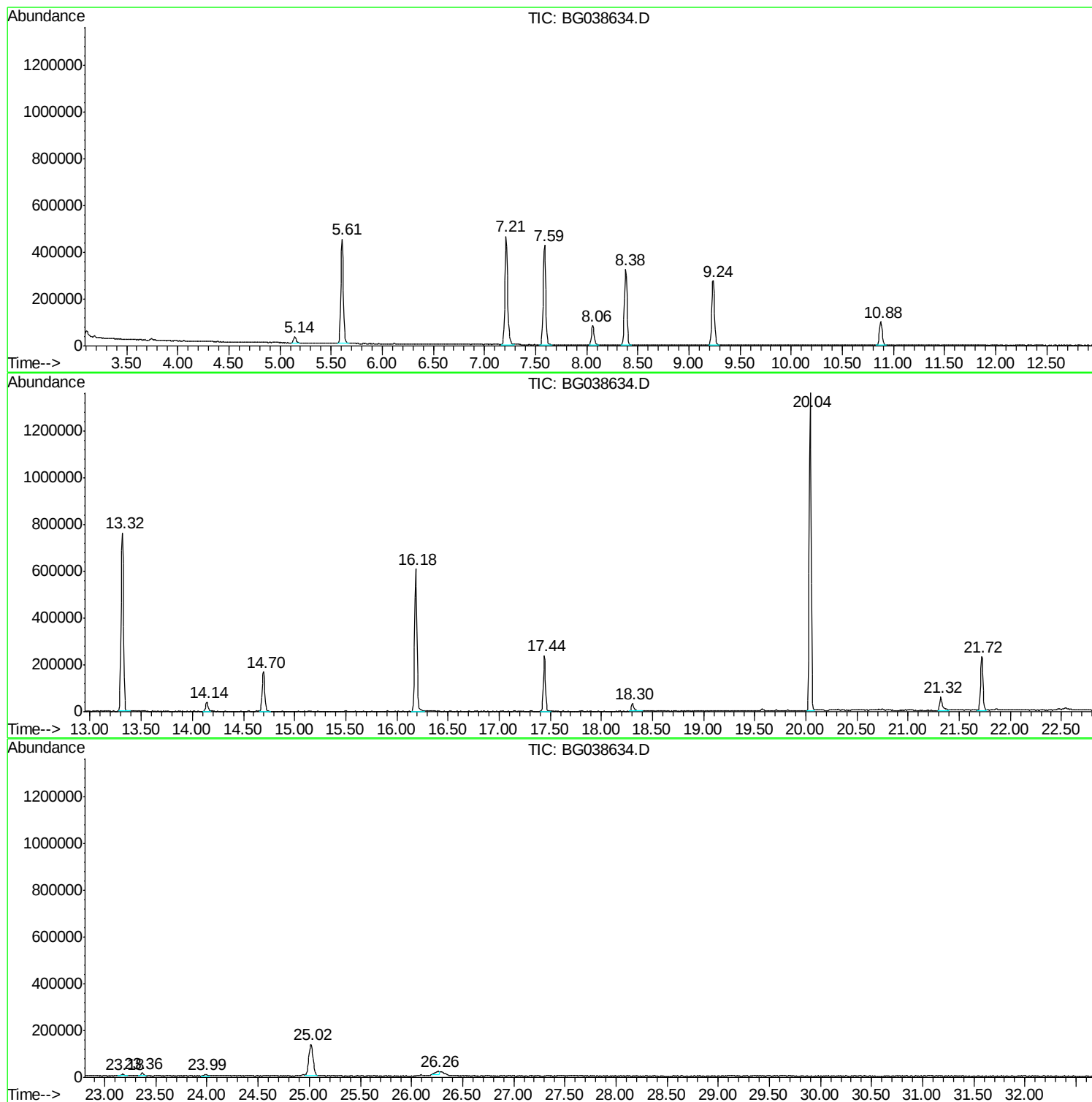
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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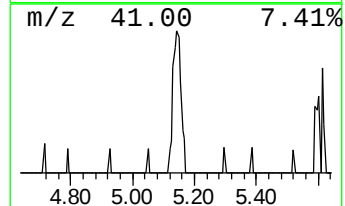
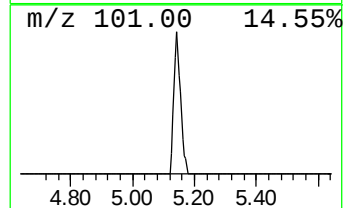
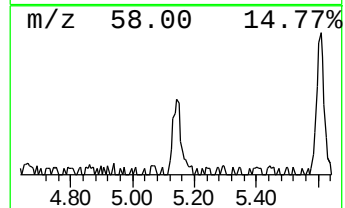
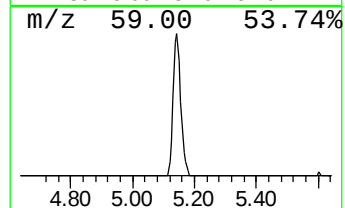
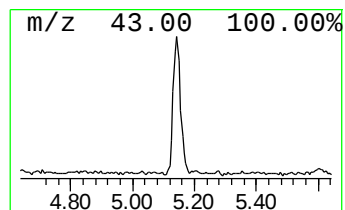
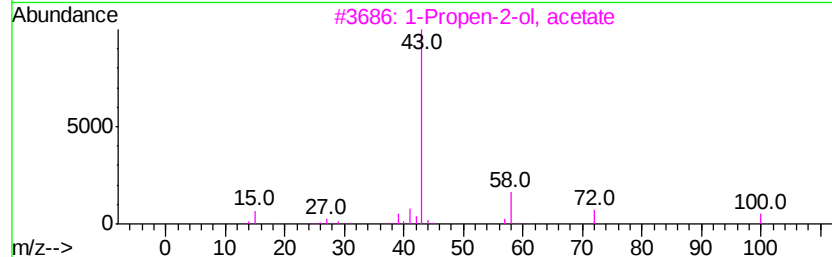
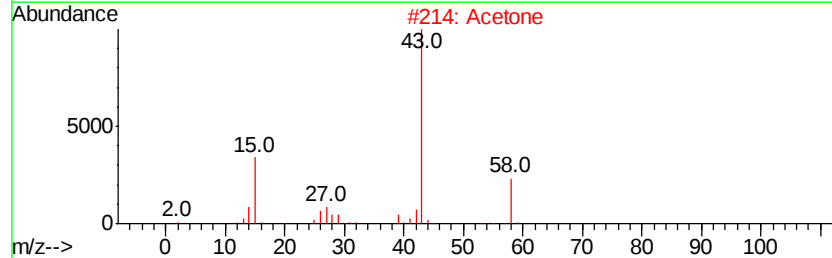
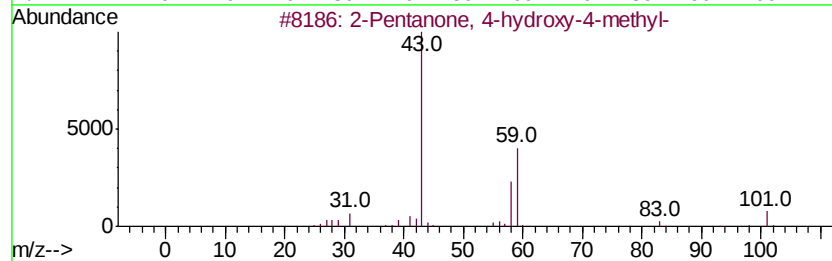
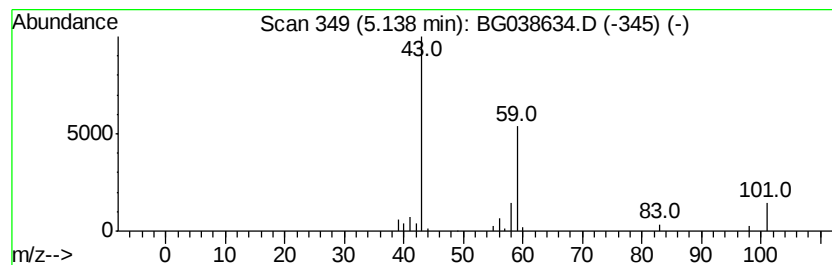
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.14 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	6.02 ng	42527	1,4-Dichlorobenzene-d4	8.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Acetone	58	C3H6O	000067-64-1	9
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	7
5			Diacetamide	101	C4H7NO2	000625-77-4	7



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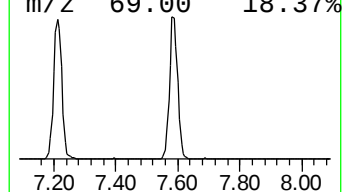
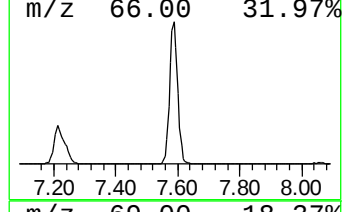
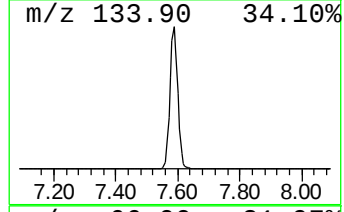
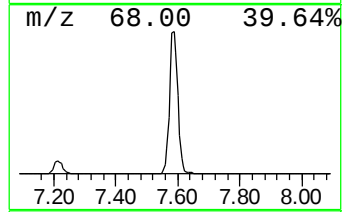
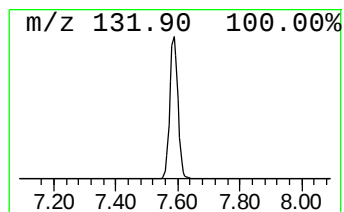
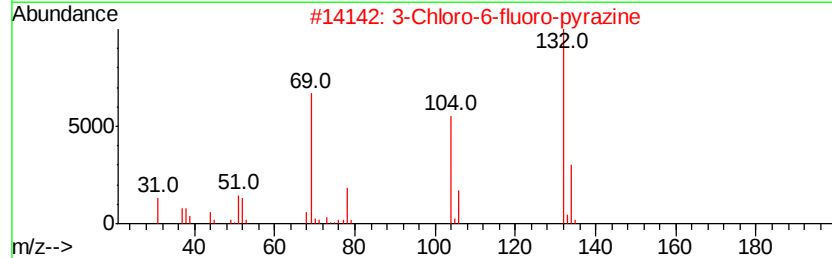
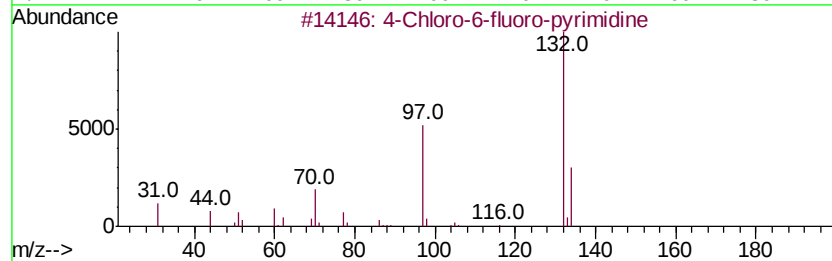
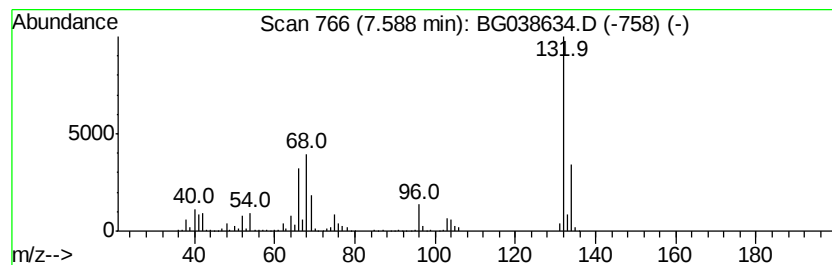
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
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Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	108.33 ng	765076	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	22
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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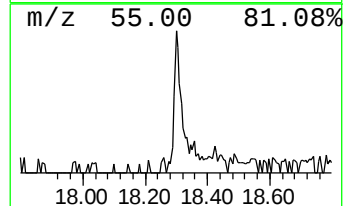
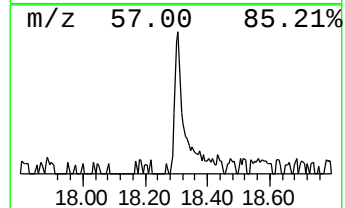
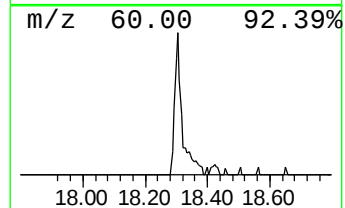
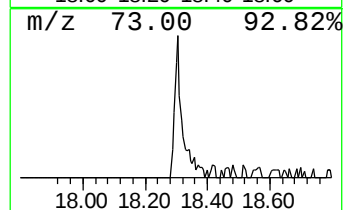
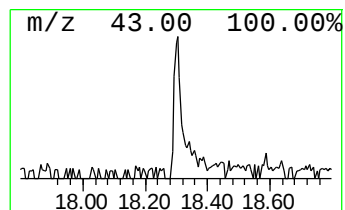
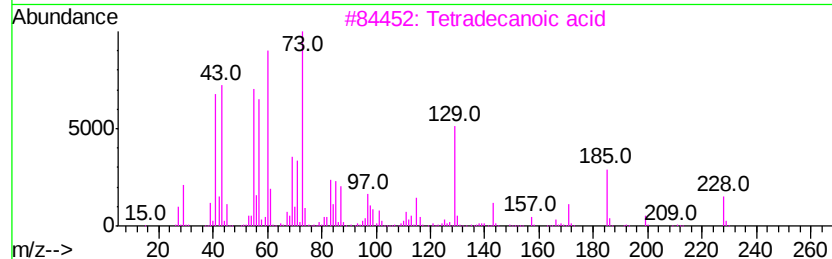
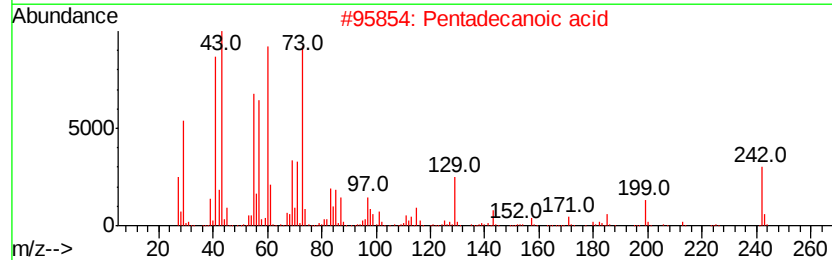
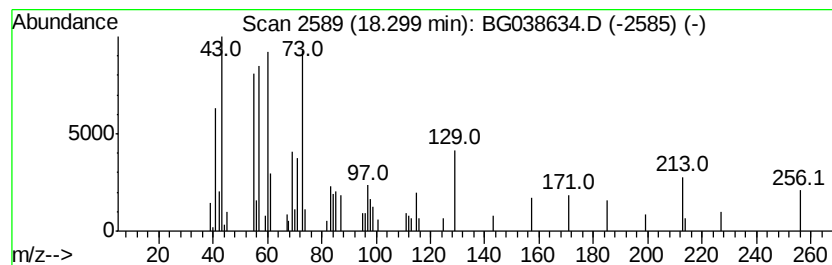
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.23 ng	58689	Phenanthrene-d10	17.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53



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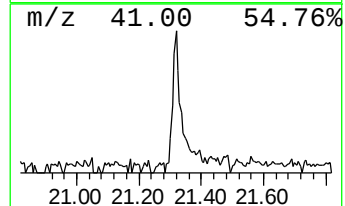
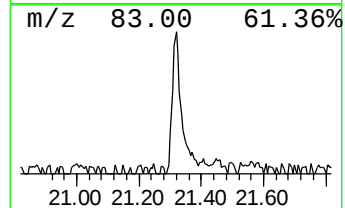
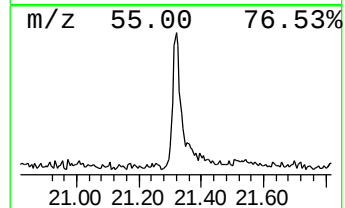
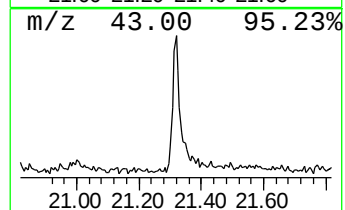
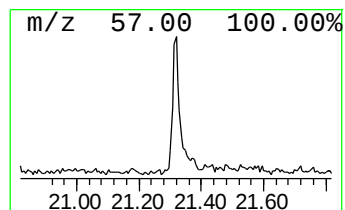
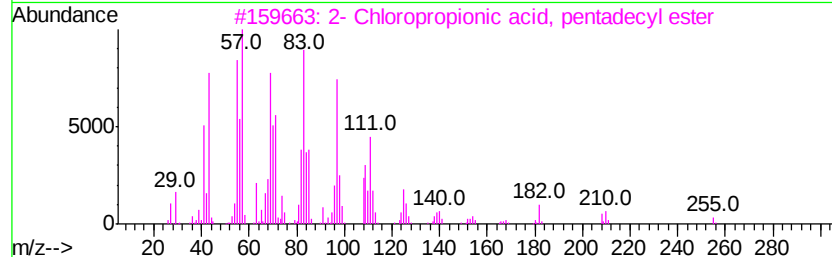
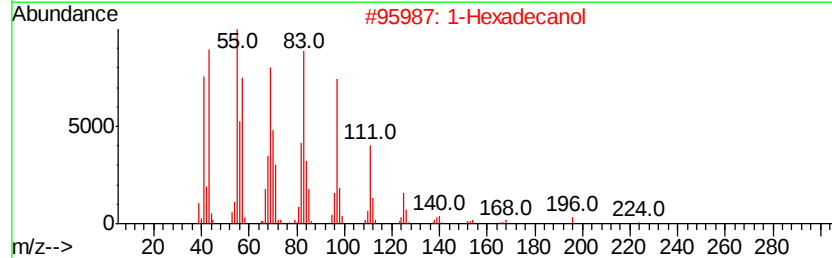
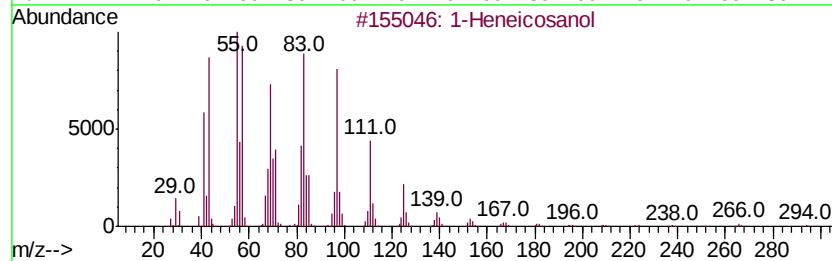
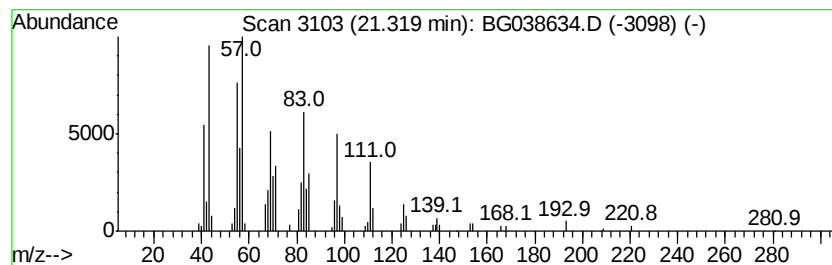
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	5.38 ng	106322	Chrysene-d12	21.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		1-Hexadecanol	242	C16H34O	036653-82-4	91
3		2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
4		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	91



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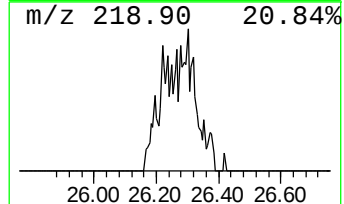
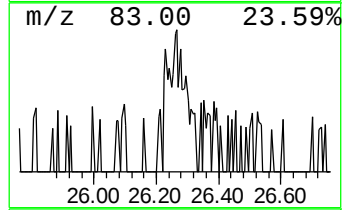
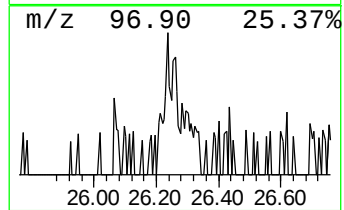
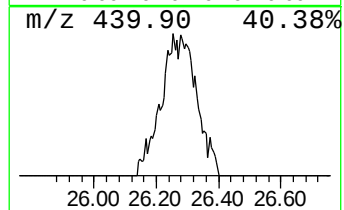
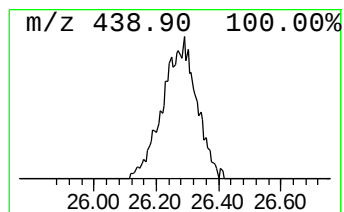
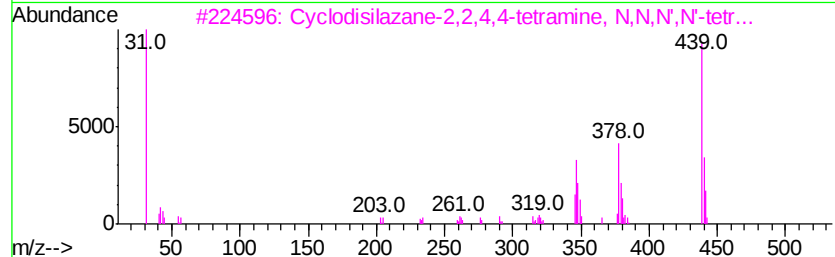
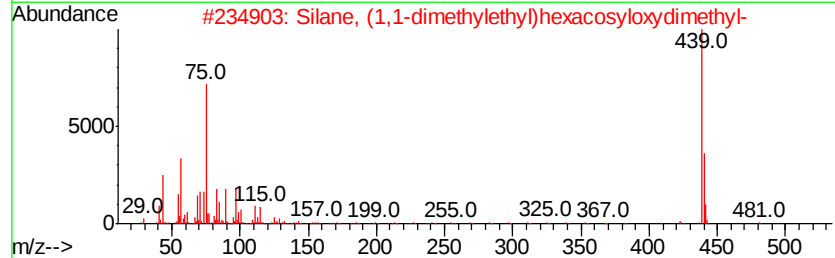
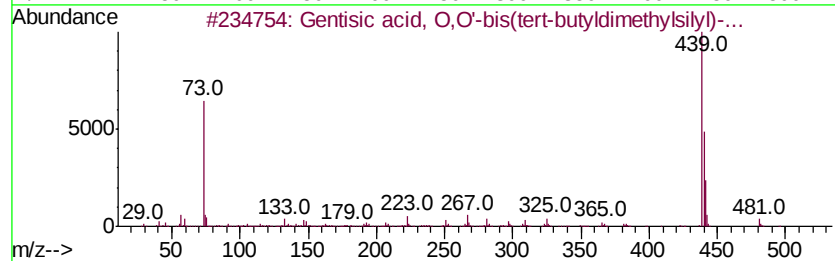
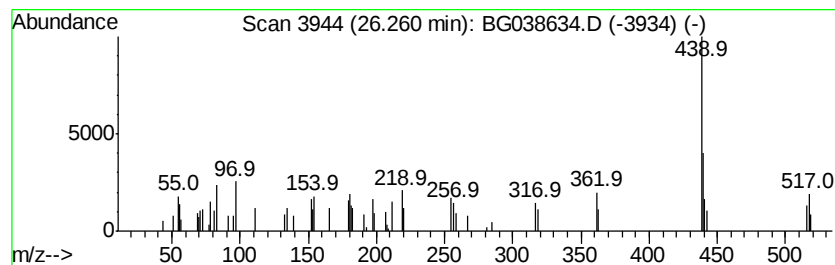
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Peak Number 6 unknown26.26 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.26	2.09 ng	40505	Perylene-d12	25.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Gentisic acid, O,O'-bis(tert-but...	496	C25H48O4Si3	1000332-90-2	38
2		Silane, (1,1-dimethylethyl)hexac...	497	C32H68OSi	1000351-85-6	38
3		Cyclodisilazane-2,2,4,4-tetramin...	440	C10H40N12Si4	034665-55-9	38
4		3,4-Dihydroxybenzoic acid, bis(t...	496	C25H48O4Si3	1000352-46-7	38
5		5-(4-Chlorophenyl)-6-ethylpyrimi...	440	C16H11ClF6N4O2	1000373-24-2	28



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown5.14	5.14	6.0	ng	42527	1	8.06	141250	20.0
unknown7.59	7.59	108.3	ng	765076	1	8.06	141250	20.0
n-Hexadecanoic acid	18.30	3.2	ng	58689	4	17.44	362846	20.0
1-Heneicosanol	21.32	5.4	ng	106322	5	21.72	395353	20.0
unknown26.26	26.26	2.1	ng	40505	6	25.02	388396	20.0