

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA G\DATA\BG062217\
 Data File : BG027603.D
 Acq On : 22 Jun 2017 19:34
 Operator : SJ/JU
 Sample : I3799-13
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-08-11.5-12.0

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-BG062117.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	5.639	292	298	310	rBV	56329	94562	5.14%	1.104%
2	6.085	366	374	383	rBV	322588	556855	30.29%	6.499%
3	7.642	629	639	648	rBV	317731	594202	32.32%	6.935%
4	8.036	699	706	717	rVB	324229	582397	31.68%	6.797%
5	8.506	779	786	794	rBB	65038	116257	6.32%	1.357%
6	8.829	832	841	850	rBB	227927	407089	22.14%	4.751%
7	9.669	976	984	993	rBV	179601	344406	18.73%	4.020%
8	11.320	1257	1265	1273	rBV	87588	172468	9.38%	2.013%
9	13.712	1660	1672	1680	rBV	530839	859977	46.78%	10.037%
10	14.516	1804	1809	1815	rBV	52320	79274	4.31%	0.925%
11	15.086	1899	1906	1916	rVB2	153232	257174	13.99%	3.002%
12	16.573	2152	2159	2169	rBV	524026	844655	45.95%	9.858%
13	17.836	2365	2374	2384	rVB2	242639	391765	21.31%	4.572%
14	18.670	2512	2516	2526	rBV	35906	59236	3.22%	0.691%
15	19.928	2726	2730	2737	rBV2	18555	28783	1.57%	0.336%
16	20.075	2749	2755	2760	rBV2	21754	26269	1.43%	0.307%
17	20.415	2806	2813	2819	rBV	1298024	1838327	100.00%	21.456%
18	21.755	3036	3041	3054	rBV5	28894	67183	3.65%	0.784%
19	22.202	3110	3117	3127	rVB	259523	477575	25.98%	5.574%
20	25.633	3676	3701	3703	rBV4	68157	304914	16.59%	3.559%
21	25.839	3725	3736	3750	rVB2	136198	464713	25.28%	5.424%

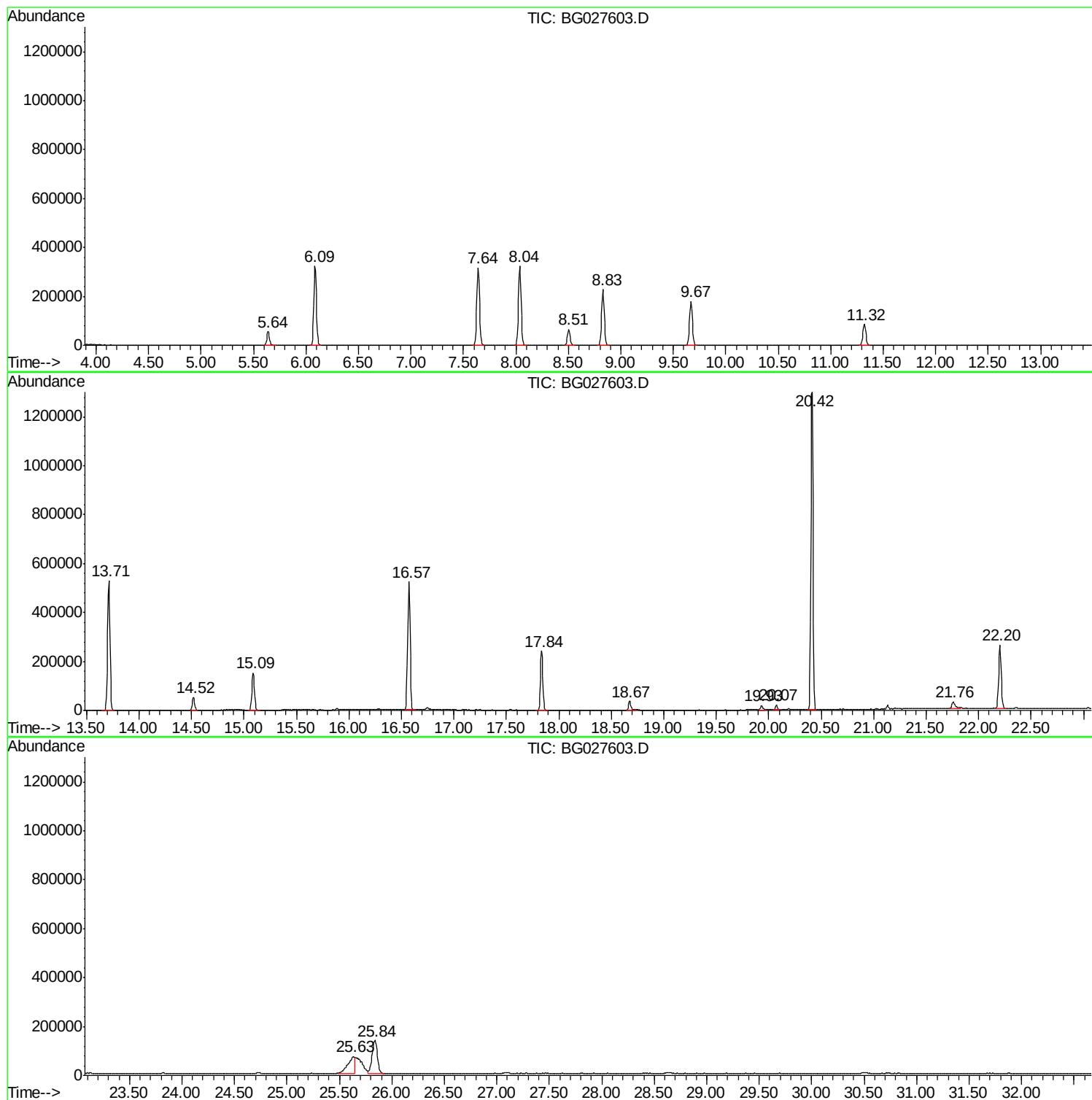
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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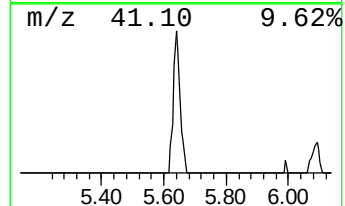
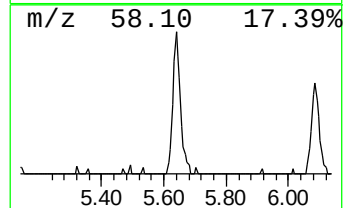
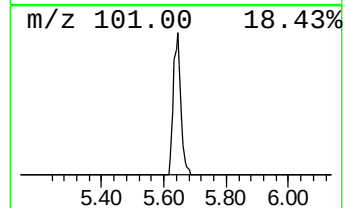
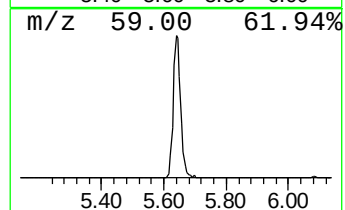
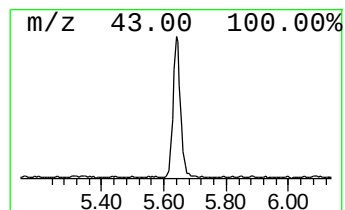
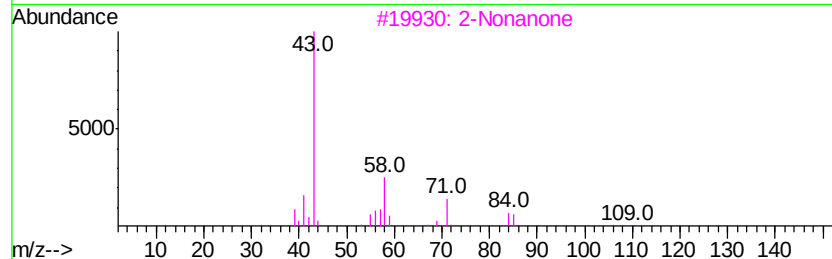
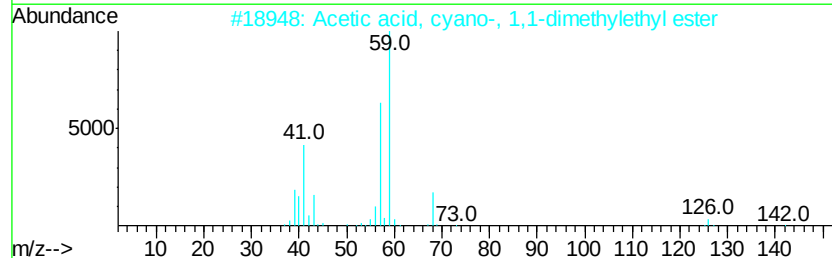
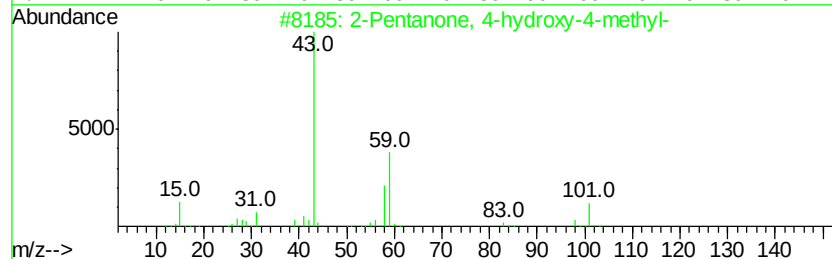
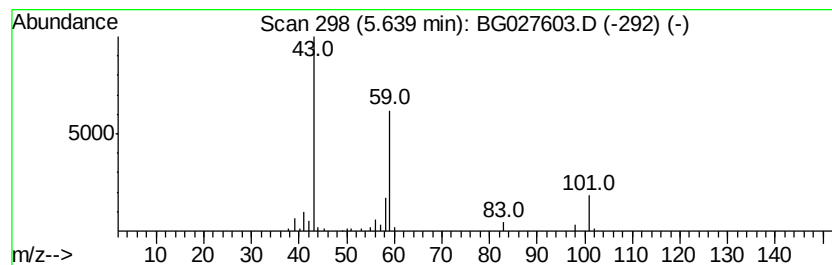
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.64	16.27 ng	94562	1,4-Dichlorobenzene-d4	8.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			2-Nonanone	142	C9H18O	000821-55-6	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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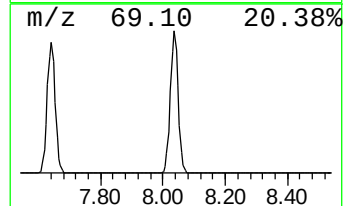
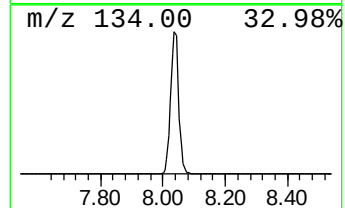
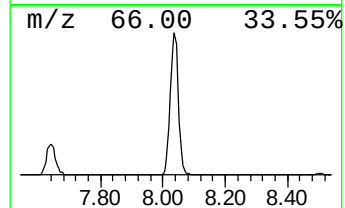
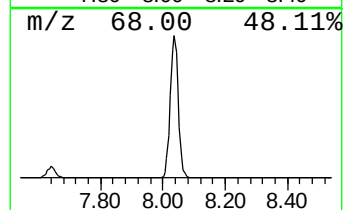
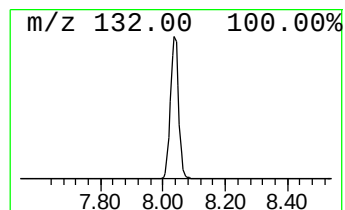
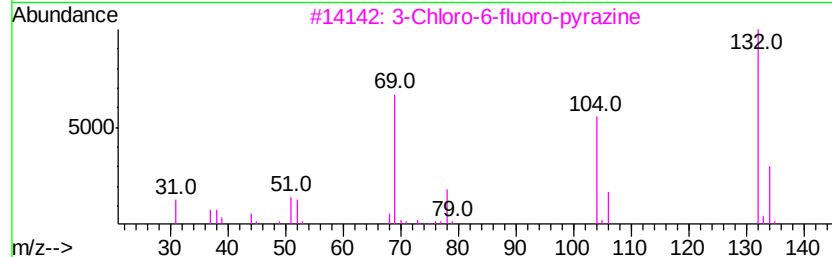
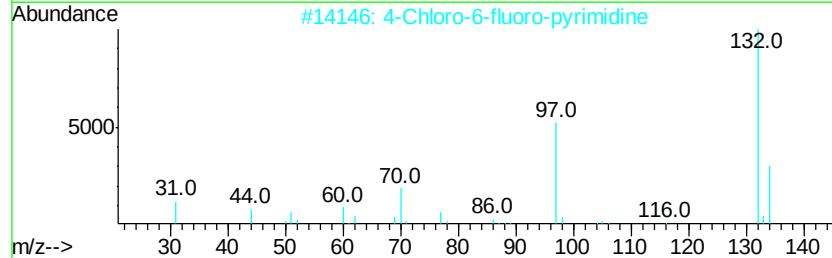
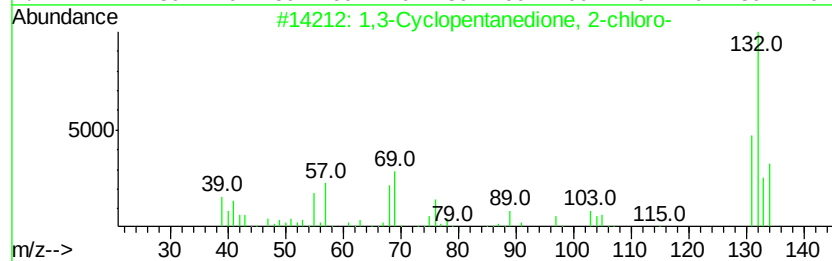
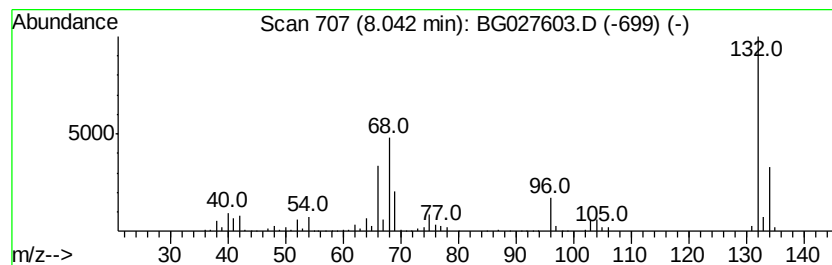
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Peak Number 2 unknown8.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.04	100.19 ng	582397	1,4-Dichlorobenzene-d4	8.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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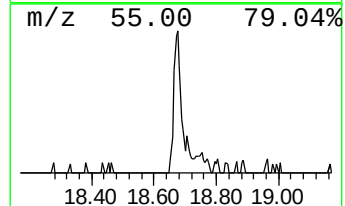
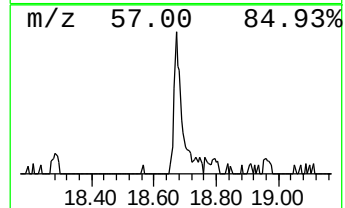
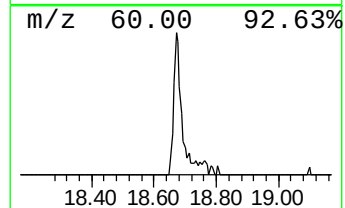
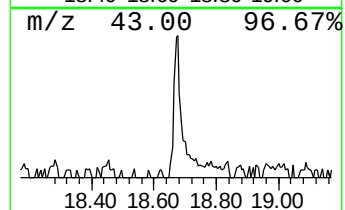
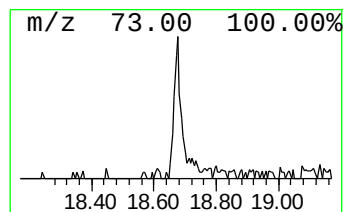
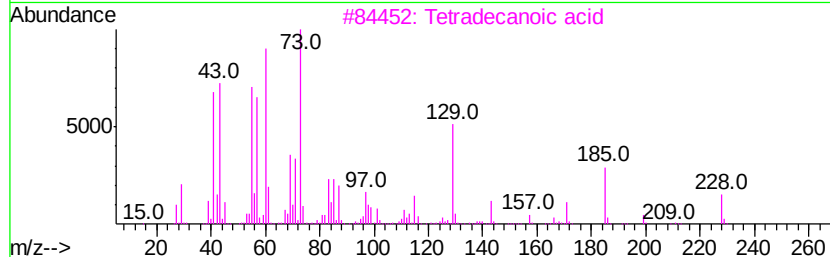
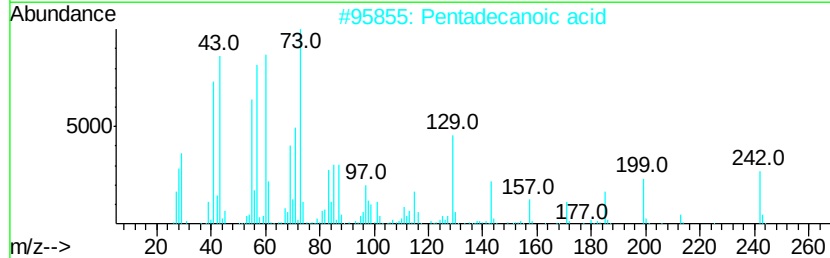
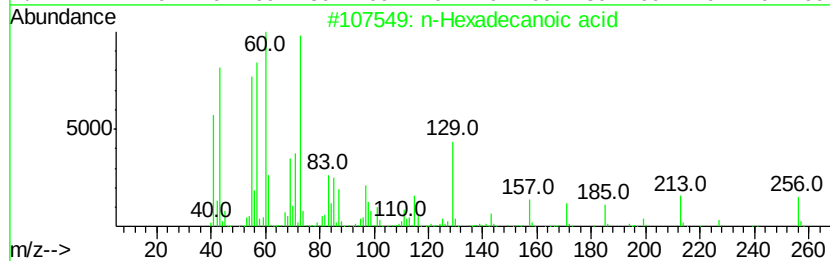
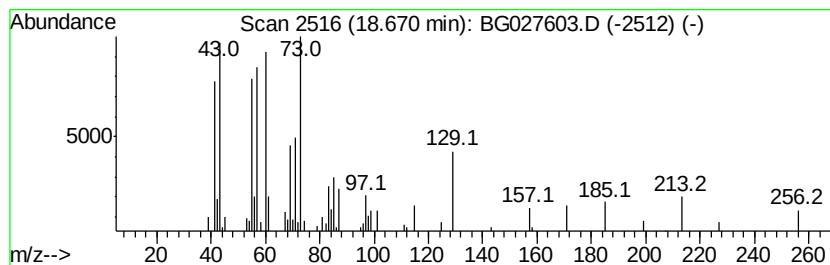
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.67	3.02 ng	59236	Phenanthrene-d10	17.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50
5	Tridecanoic acid	214	C13H26O2	000638-53-9	50



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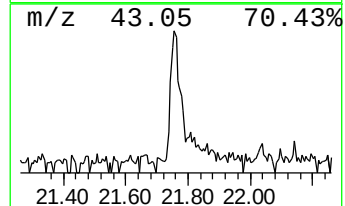
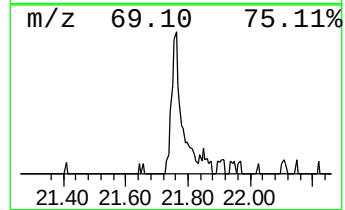
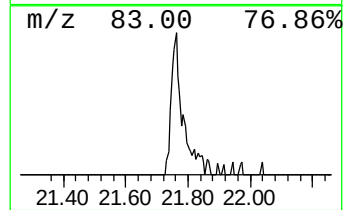
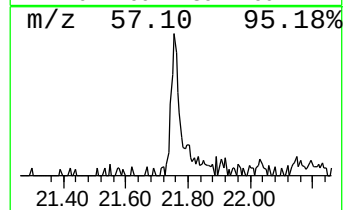
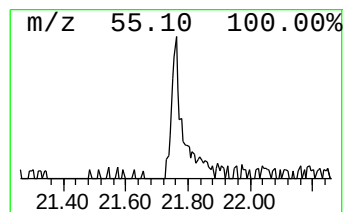
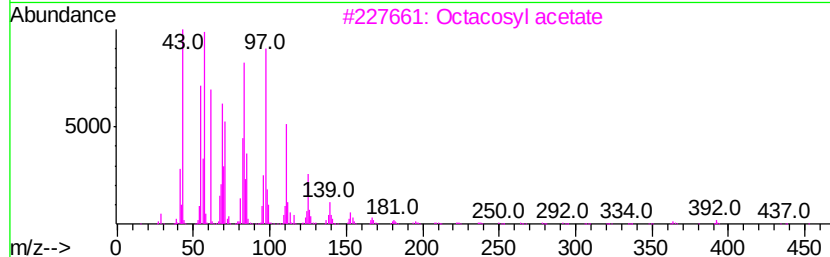
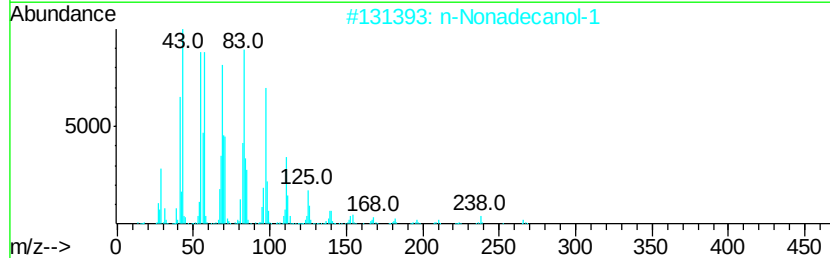
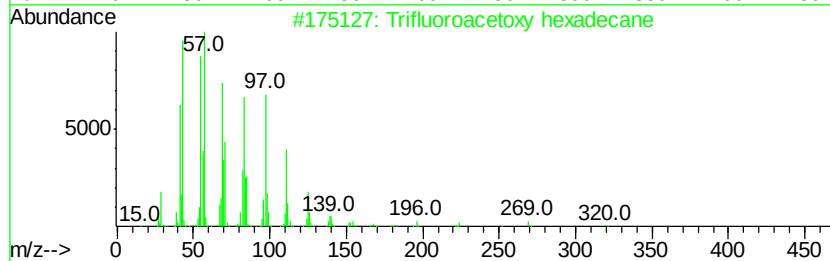
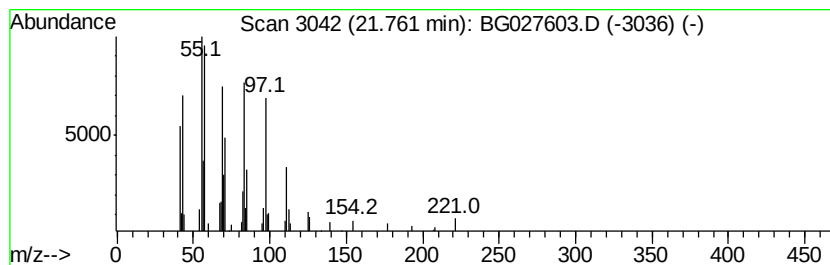
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.76	2.81 ng	67183	Chrysene-d12	22.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3	Octacosyl acetate	452	C30H60O2	018206-97-8	87
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87



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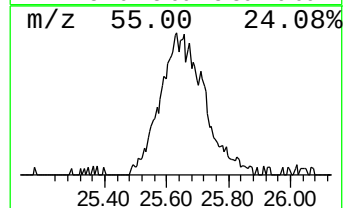
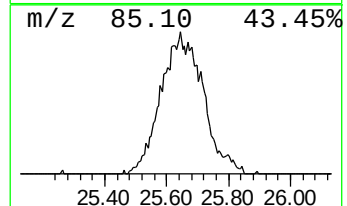
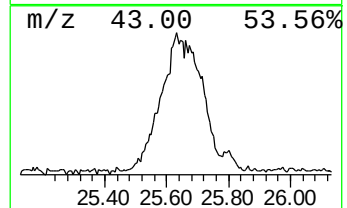
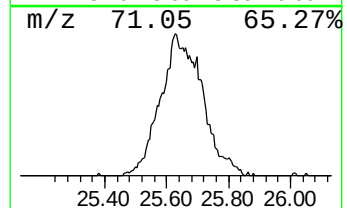
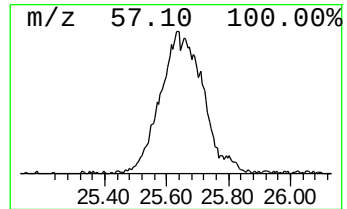
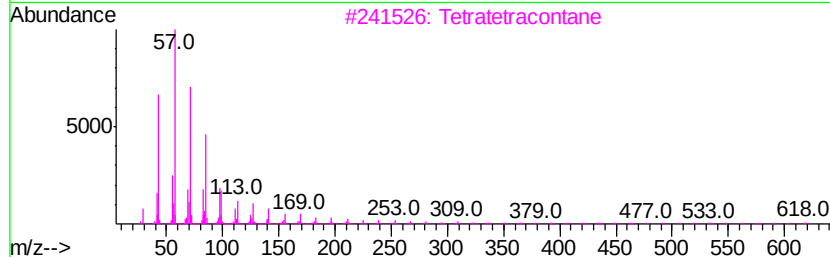
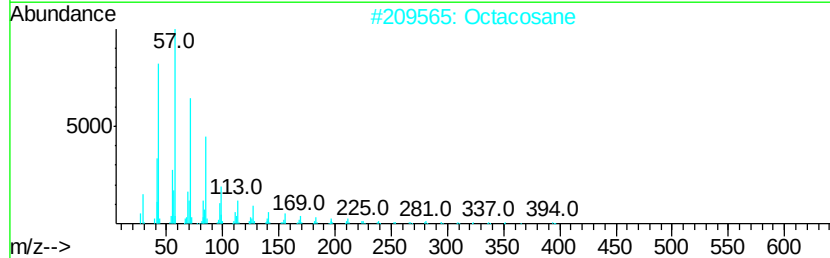
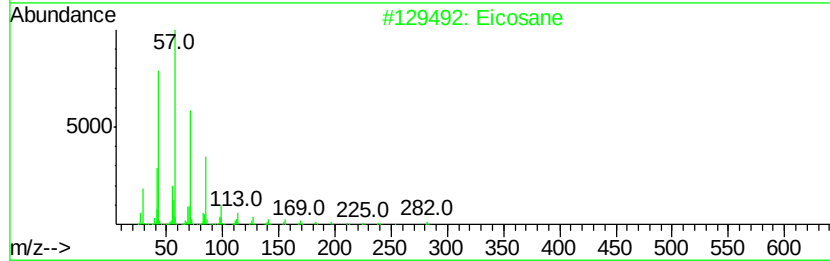
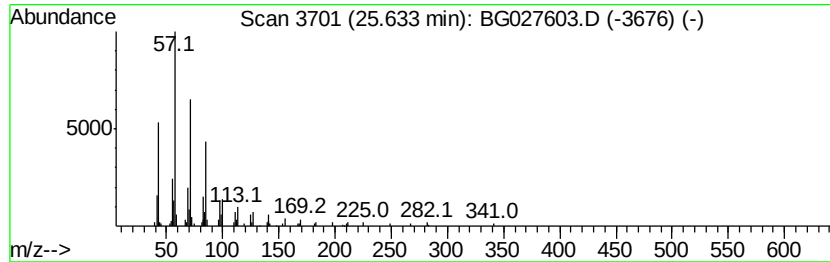
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Peak Number 6 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.63	13.12 ng	304914	Perylene-d12	25.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Octacosane	394	C28H58	000630-02-4	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		triacontane	422	C30H62	000638-68-6	90
5		2-methyloctacosane	408	C29H60	1000376-72-8	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.64	16.3	ng	94562	1	8.51	116257	20.0
unknown8.04	8.04	100.2	ng	582397	1	8.51	116257	20.0
n-Hexadecanoic acid	18.67	3.0	ng	59236	4	17.84	391765	20.0
Trifluoroacetoxy ...	21.76	2.8	ng	67183	5	22.20	477575	20.0
Eicosane	25.63	13.1	ng	304914	6	25.84	464713	20.0