

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062117\
 Data File : BG027590.D
 Acq On : 22 Jun 2017 11:01
 Operator : SJ/JU
 Sample : I3799-03
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-03-9.5-10.0

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-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	5.638	292	298	306	rBV	65791	111164	5.17%	1.110%
2	6.085	367	374	387	rBV	402362	680782	31.68%	6.799%
3	7.642	631	639	648	rBV	406953	750120	34.90%	7.492%
4	8.035	699	706	716	rBV	392770	705869	32.84%	7.050%
5	8.505	778	786	795	rBB	84954	149983	6.98%	1.498%
6	8.829	834	841	849	rBV	268155	490108	22.80%	4.895%
7	9.669	974	984	995	rBV	224267	438441	20.40%	4.379%
8	11.320	1258	1265	1273	rVB	122424	225025	10.47%	2.247%
9	13.711	1662	1672	1680	rBV	669878	1066712	49.63%	10.654%
10	14.522	1802	1810	1815	rBV	56728	88811	4.13%	0.887%
11	15.086	1900	1906	1914	rBV3	196421	332913	15.49%	3.325%
12	16.572	2152	2159	2172	rBV	677911	1038348	48.31%	10.370%
13	17.836	2367	2374	2380	rBV	314555	504505	23.47%	5.039%
14	18.676	2512	2517	2528	rBV	36418	59062	2.75%	0.590%
15	20.415	2807	2813	2819	rBV	1629941	2149260	100.00%	21.465%
16	21.755	3036	3041	3050	rBV3	30869	65847	3.06%	0.658%
17	22.201	3110	3117	3126	rVB	311989	589262	27.42%	5.885%
18	25.838	3721	3736	3752	rBV3	175464	566547	26.36%	5.658%

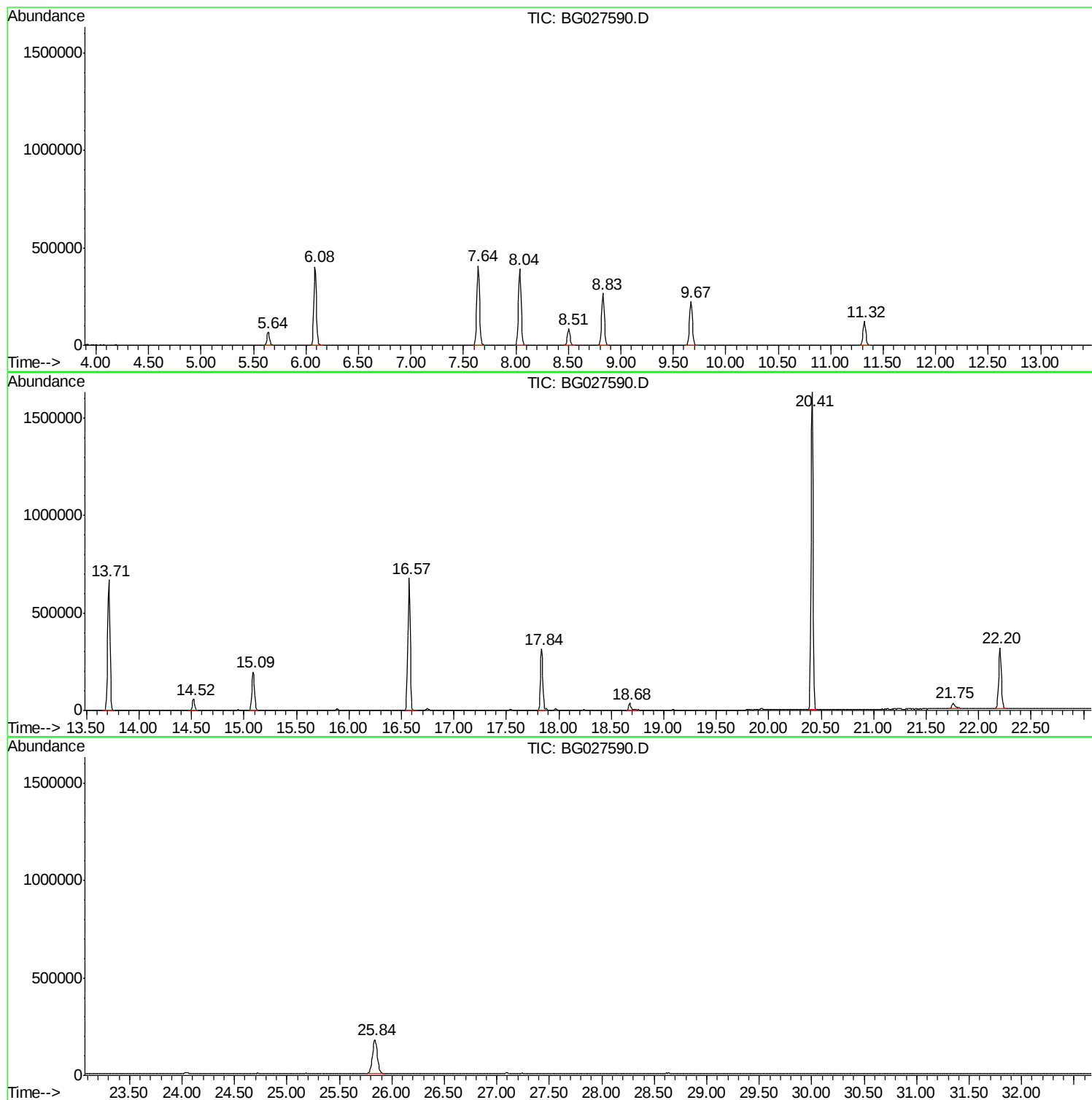
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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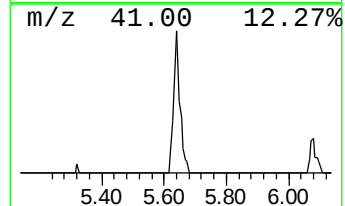
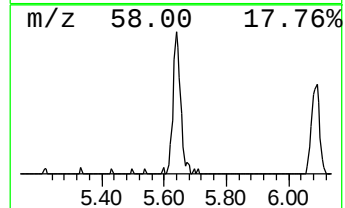
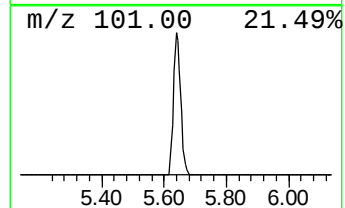
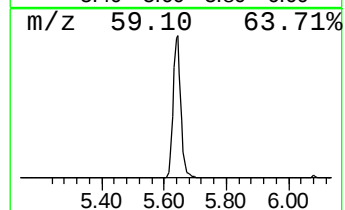
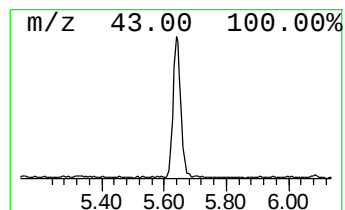
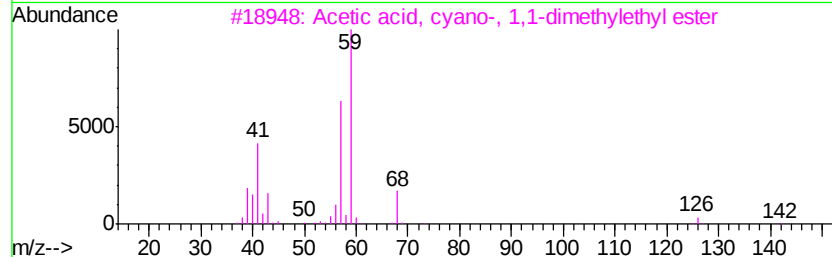
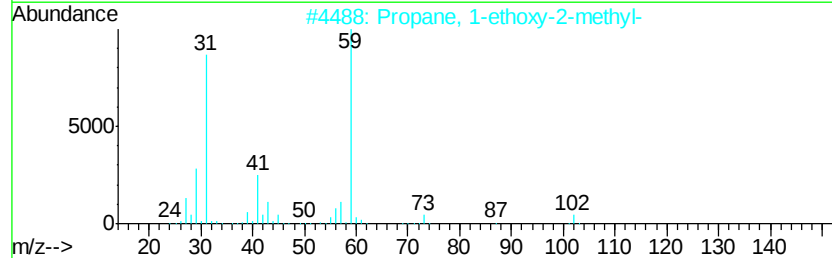
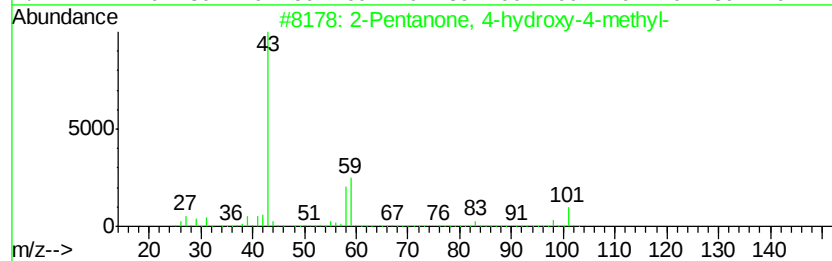
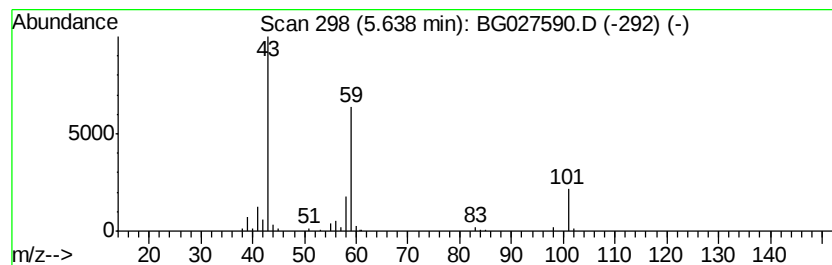
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.64	14.82 ng	111164	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	64
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	43
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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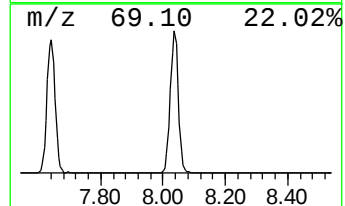
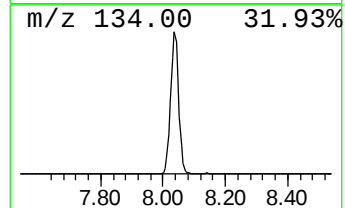
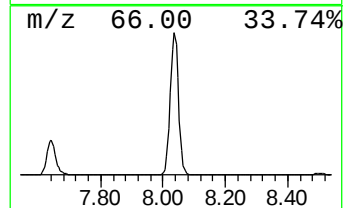
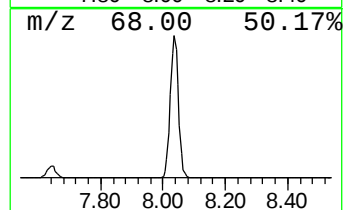
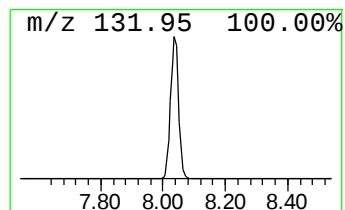
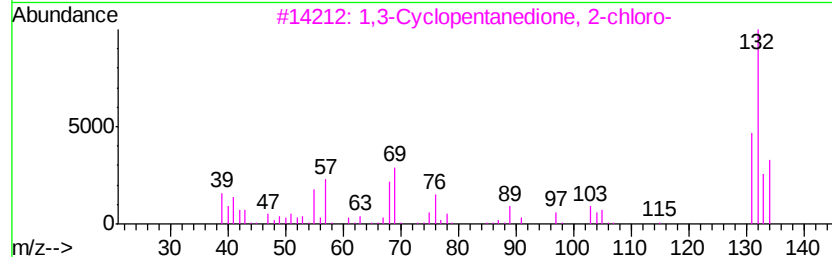
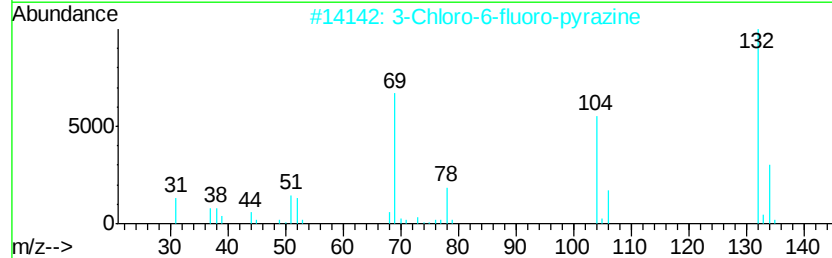
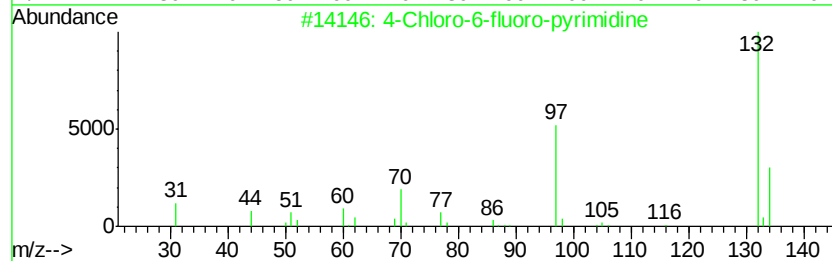
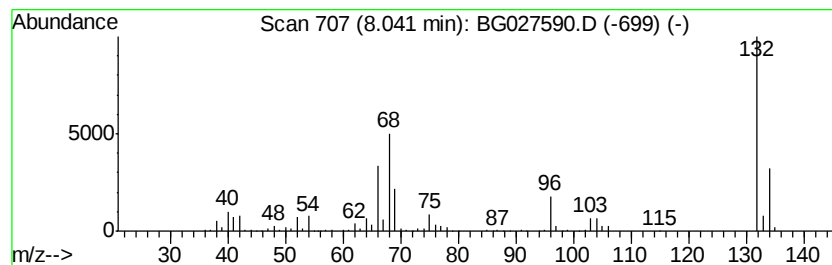
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Peak Number 2 unknown8.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.04	94.13 ng	705869	1,4-Dichlorobenzene-d4	8.51

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		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22



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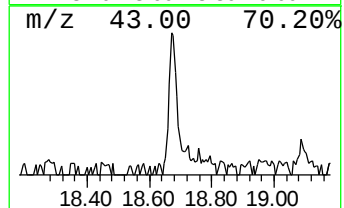
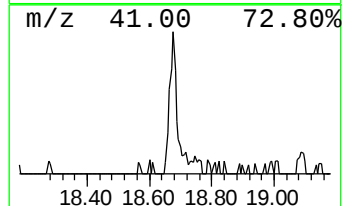
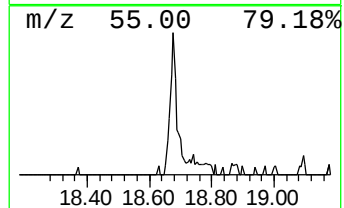
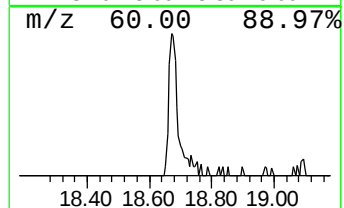
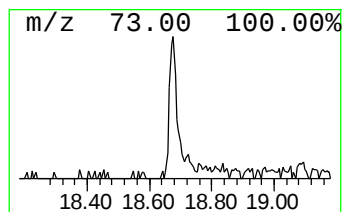
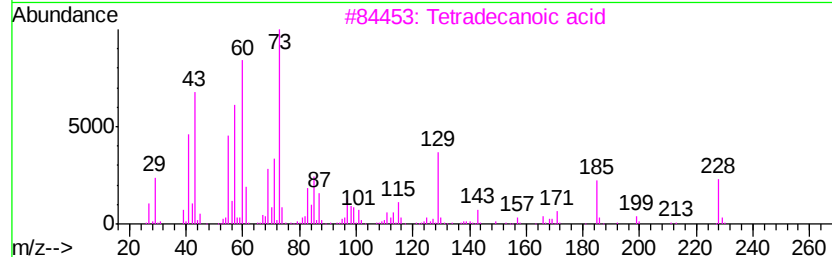
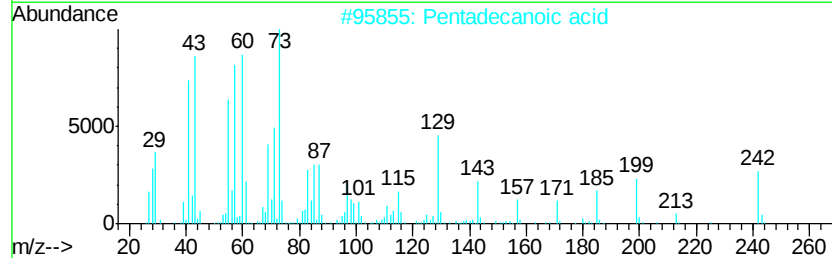
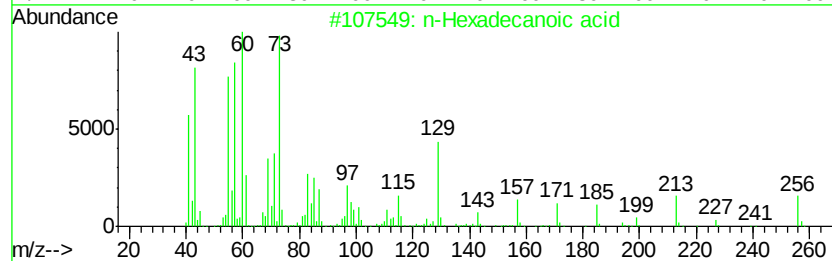
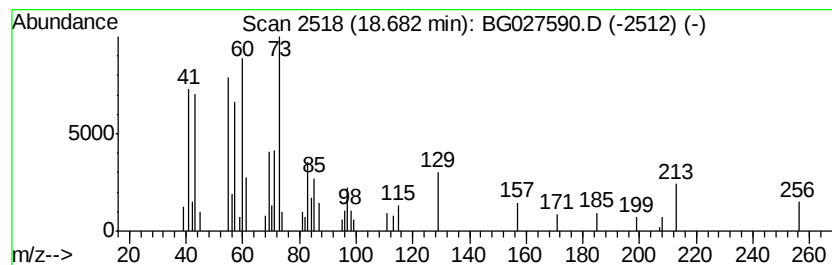
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.68	2.34 ng	59062	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	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



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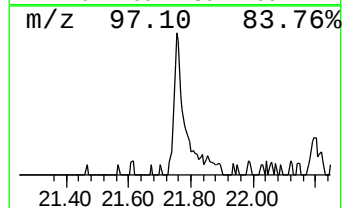
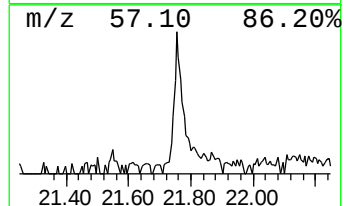
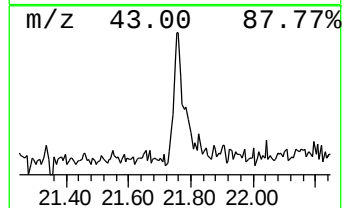
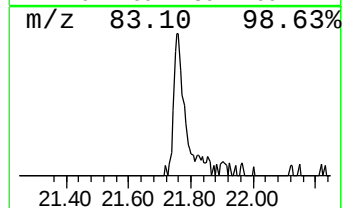
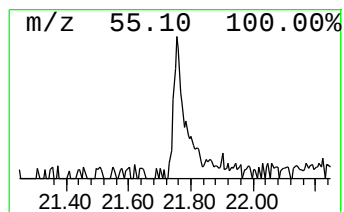
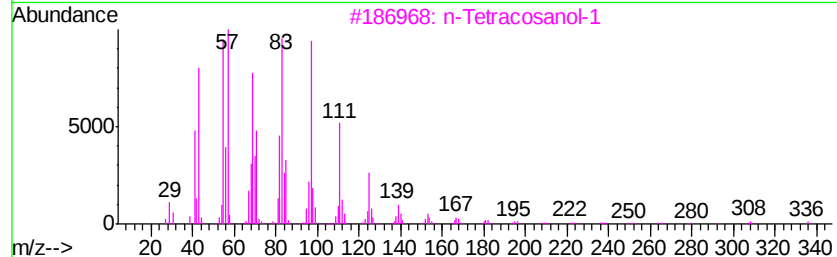
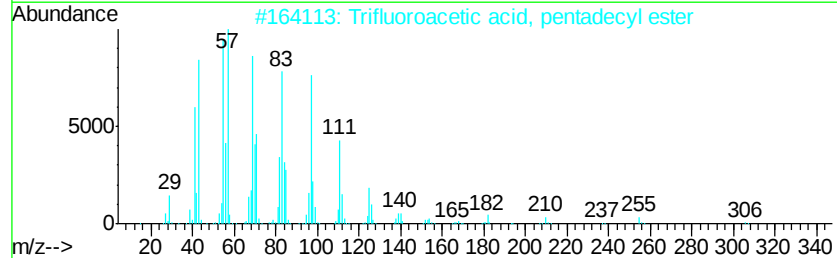
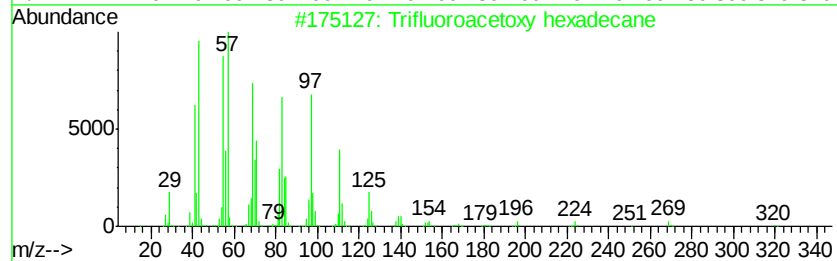
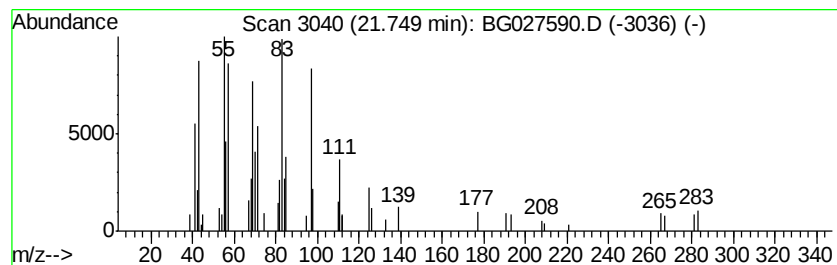
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.75	2.23 ng	65847	Chrysene-d12	22.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.64	14.8	ng	111164	1	8.51	149983	20.0
unknown8.04	8.04	94.1	ng	705869	1	8.51	149983	20.0
n-Hexadecanoic acid	18.68	2.3	ng	59062	4	17.84	504505	20.0
Trifluoroacetoxy ...	21.75	2.2	ng	65847	5	22.20	589262	20.0