

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080718\
 Data File : BM016230.D
 Acq On : 07 Aug 2018 23:18
 Operator : SJ/JU
 Sample : J4335-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 CINNAMINSON-8-3-18

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 M\METHODS\8270-BM072318.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	5.187	318	323	335	rBV	127589	200485	3.85%	0.766%
2	5.663	398	404	424	rBV	1107960	1755549	33.68%	6.711%
3	7.304	676	683	699	rBV	1222410	2043566	39.21%	7.812%
4	7.669	737	745	756	rBV	1279749	2101745	40.32%	8.034%
5	8.139	819	825	833	rBV	240100	412665	7.92%	1.578%
6	8.457	873	879	888	rVB	873037	1400591	26.87%	5.354%
7	9.322	1019	1026	1044	rBV	681466	1185393	22.74%	4.531%
8	10.951	1297	1303	1312	rBV	322224	551823	10.59%	2.109%
9	13.392	1707	1718	1731	rBV	1936842	2705084	51.90%	10.341%
10	14.227	1855	1860	1865	rBV	125294	174710	3.35%	0.668%
11	14.774	1945	1953	1960	rBV2	515585	766017	14.70%	2.928%
12	16.262	2199	2206	2213	rBV	1860962	2586554	49.62%	9.888%
13	17.509	2412	2418	2422	rBV	699782	976372	18.73%	3.732%
14	17.551	2422	2425	2430	rVB	64841	95685	1.84%	0.366%
15	18.362	2558	2563	2570	rBV2	321631	500332	9.60%	1.913%
16	19.545	2759	2764	2769	rVB	215866	299630	5.75%	1.145%
17	19.615	2773	2776	2782	rVV	126868	171300	3.29%	0.655%
18	19.903	2821	2825	2832	rVB	228165	319599	6.13%	1.222%
19	20.092	2851	2857	2862	rBV	4609309	5212467	100.00%	19.926%
20	21.309	3061	3064	3070	rVB2	255843	350844	6.73%	1.341%
21	21.639	3114	3120	3124	rBV2	1007403	1398970	26.84%	5.348%
22	23.980	3512	3518	3524	rVB	512337	949792	18.22%	3.631%

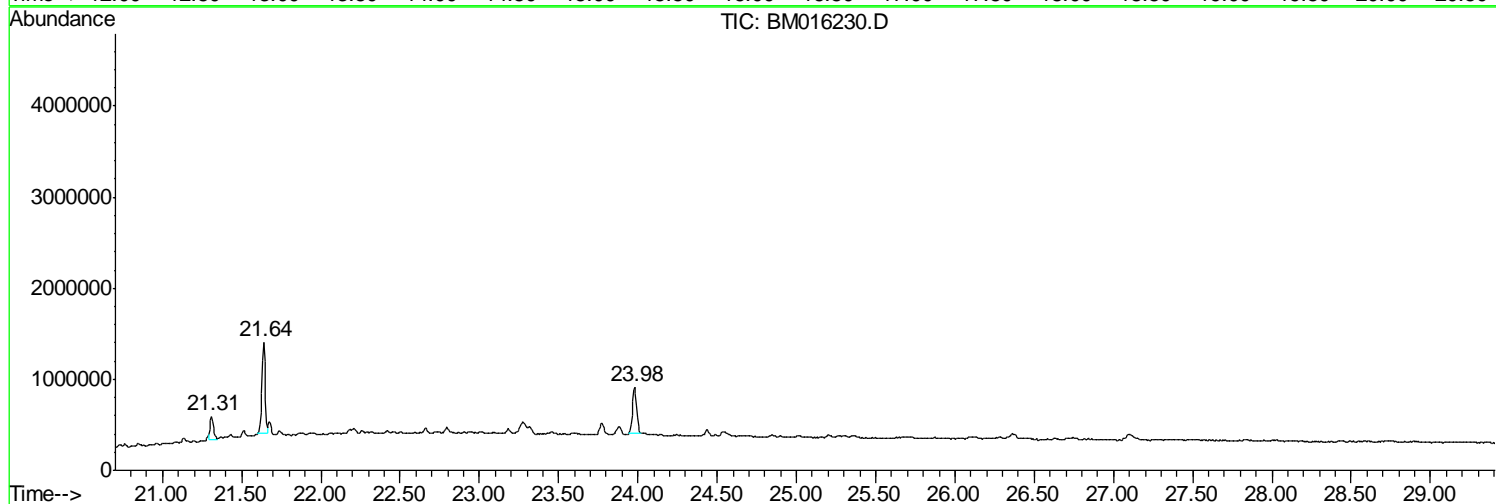
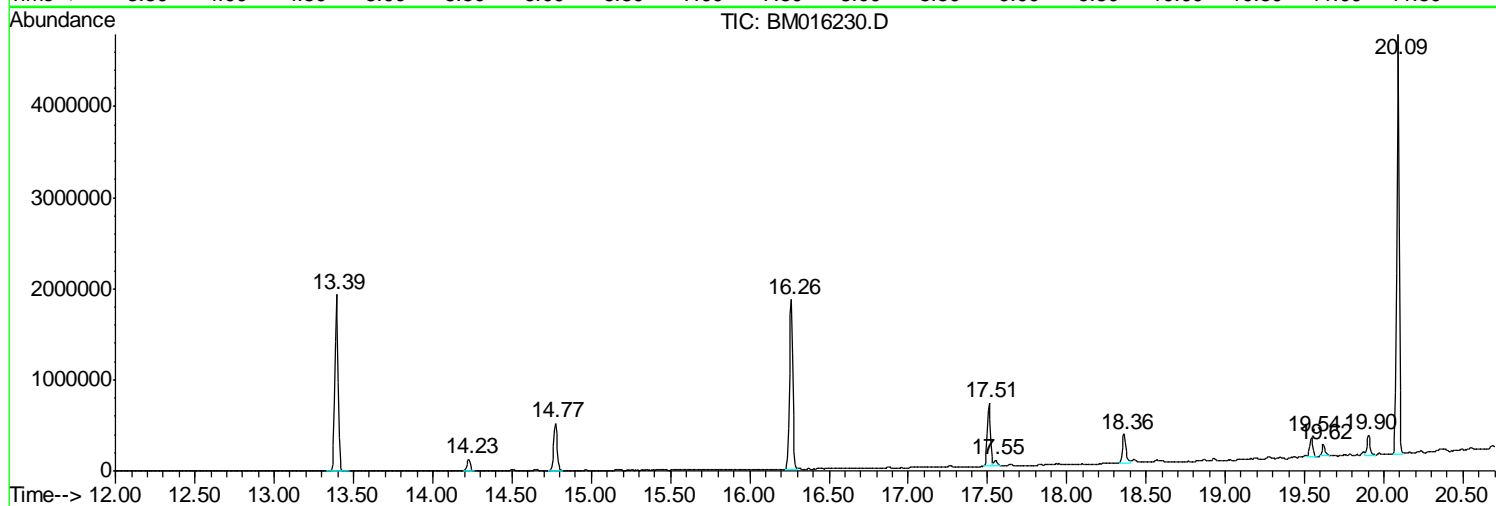
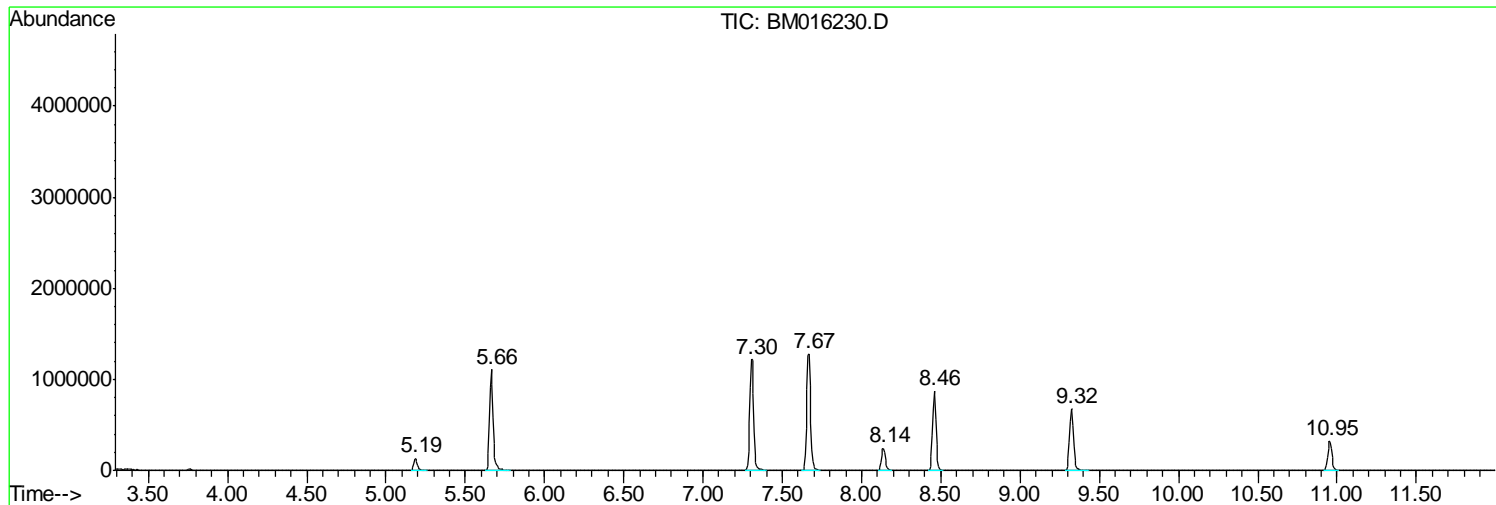
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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 ClientSampled :
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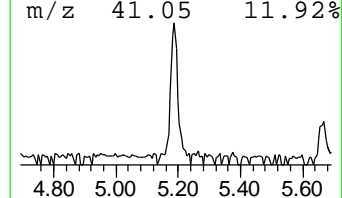
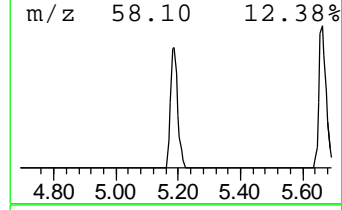
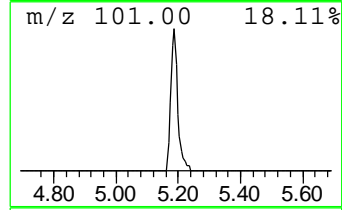
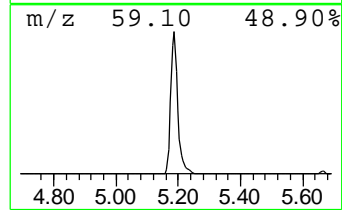
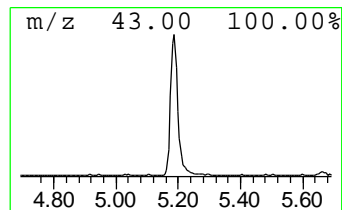
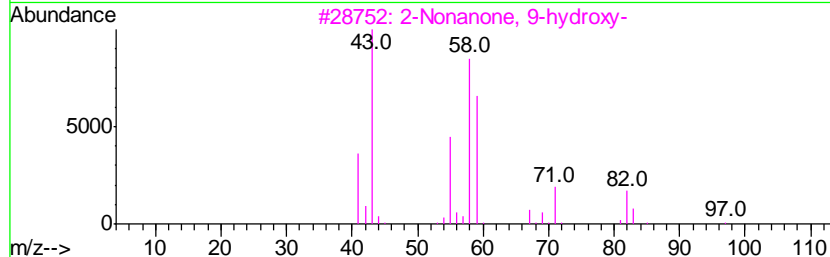
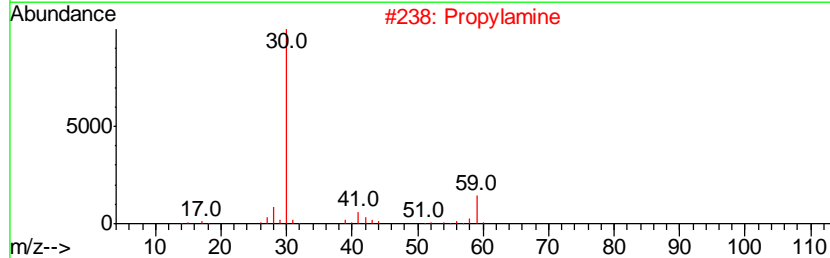
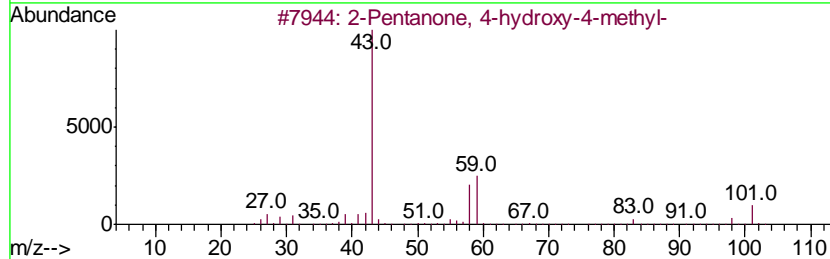
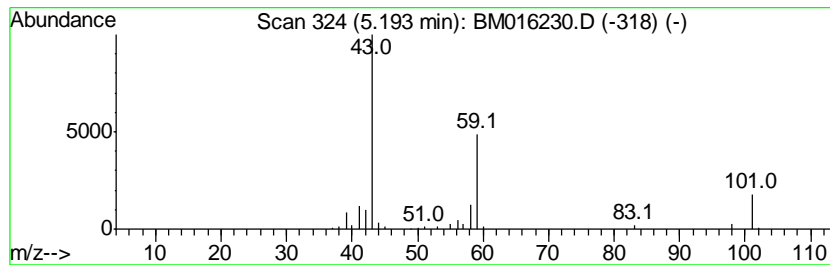
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	9.72 ng	200485	1,4-Dichlorobenzene-d4	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propylamine	59	C3H9N	000107-10-8	42
3		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27



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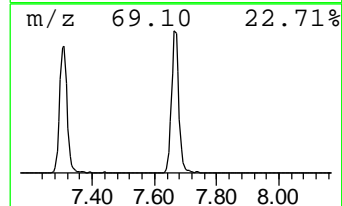
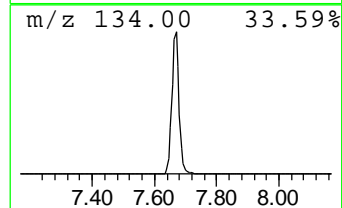
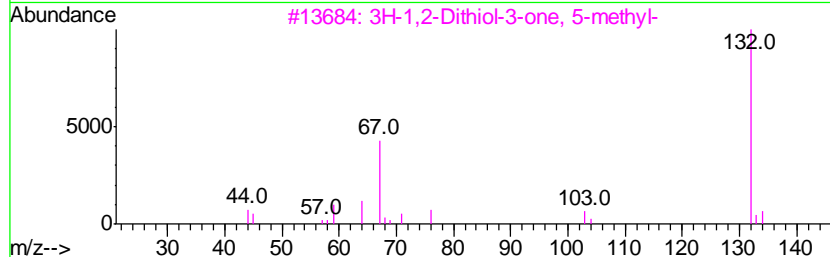
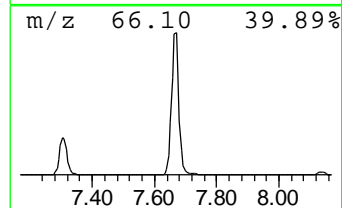
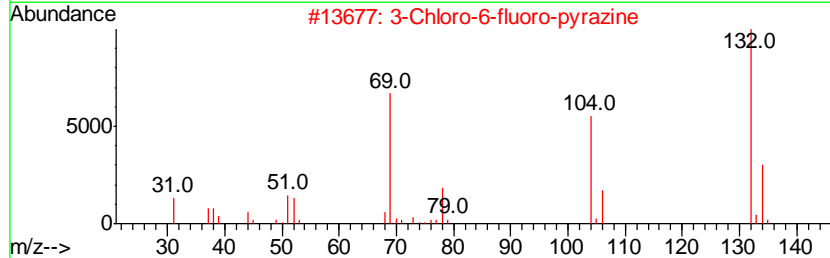
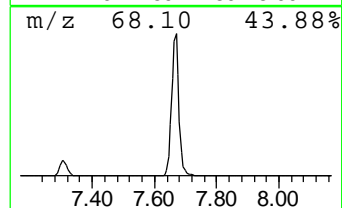
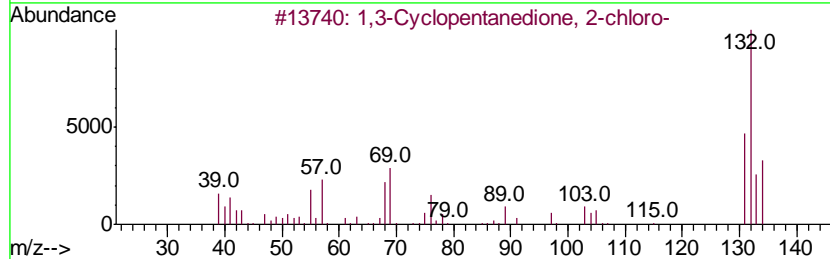
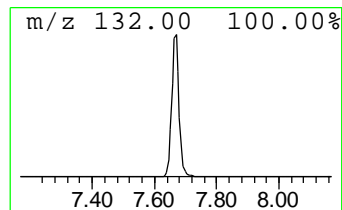
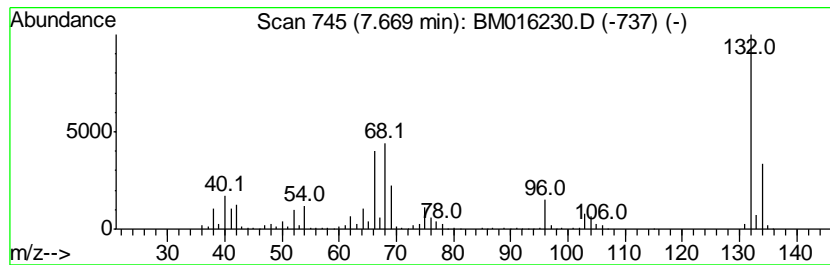
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 Peak Number 2 unknown7.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	101.86 ng	2101750	1,4-Dichlorobenzene-d4	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14



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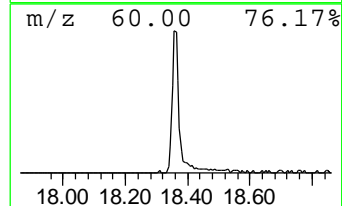
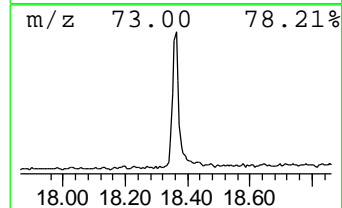
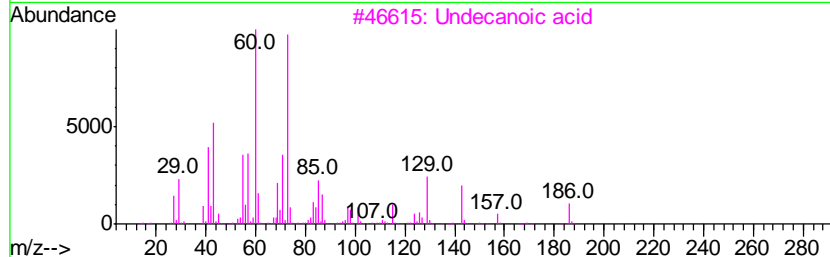
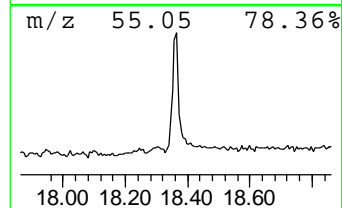
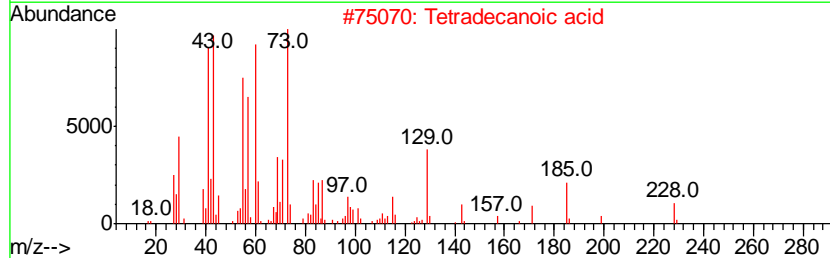
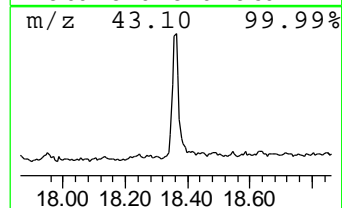
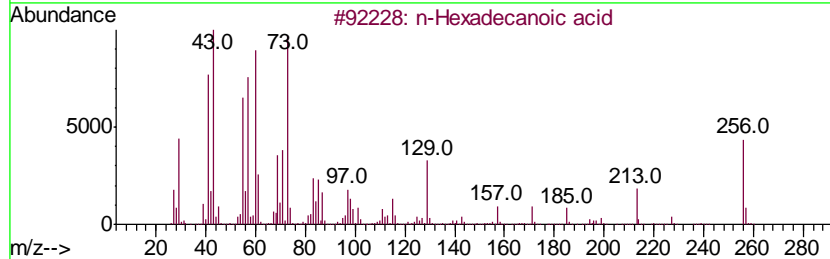
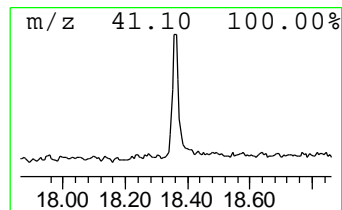
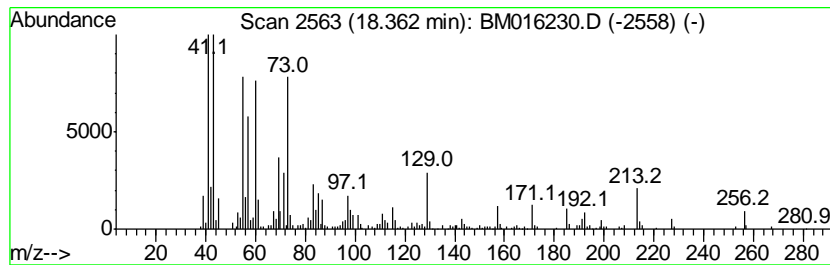
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 TIC Integration Parameters: LSCINT.P

 Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	10.25 ng	500332	Phenanthrene-d10	17.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Undecanoic acid	186	C11H22O2	000112-37-8	64
4		n-Decanoic acid	172	C10H20O2	000334-48-5	60
5		Tridecanoic acid	214	C13H26O2	000638-53-9	58



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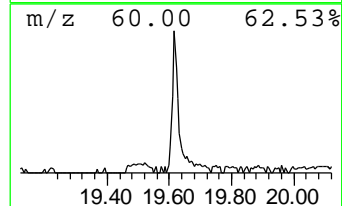
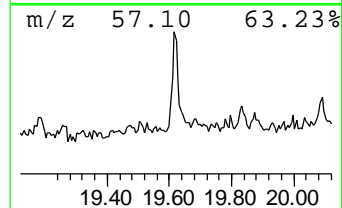
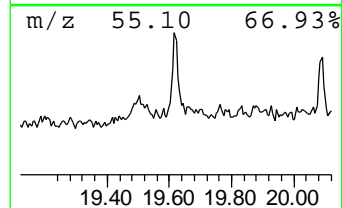
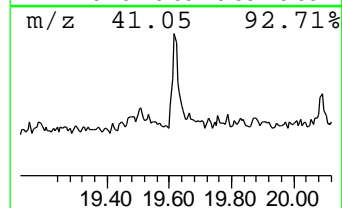
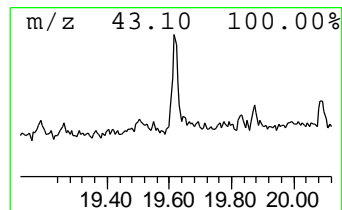
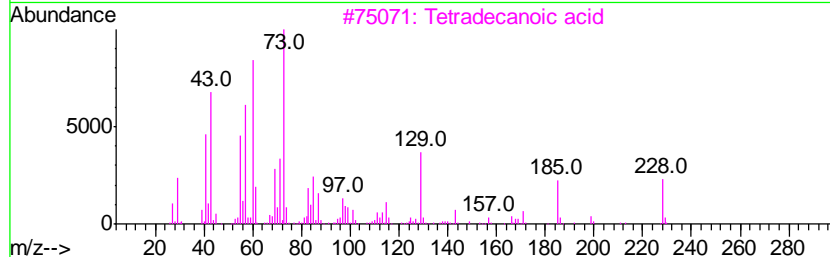
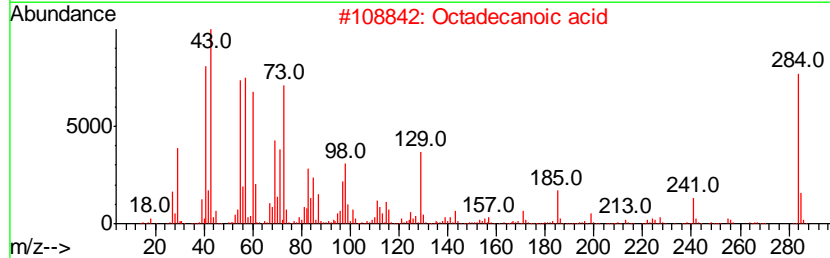
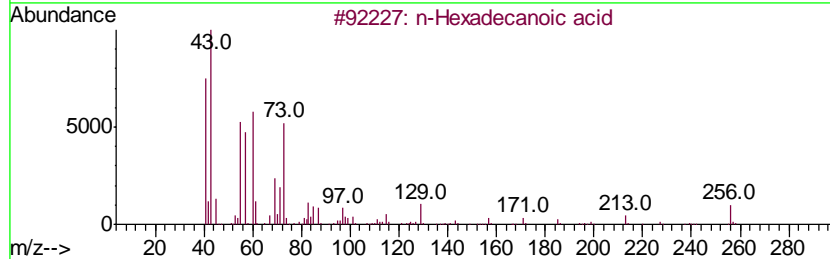
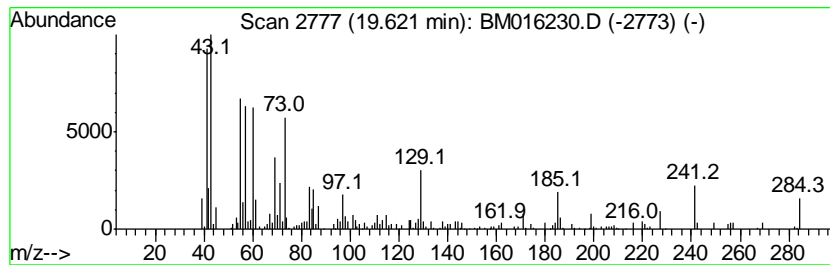
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 Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	2.45 ng	171300	Chrysene-d12	21.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2		Octadecanoic acid	284	C18H36O2	000057-11-4	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	70
4		Undecanoic acid	186	C11H22O2	000112-37-8	60
5		Heptadecanoic acid	270	C17H34O2	000506-12-7	52



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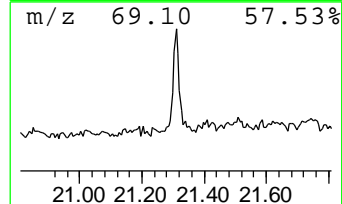
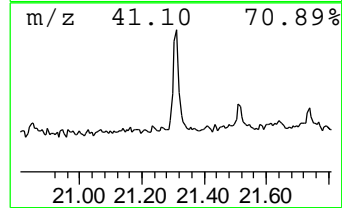
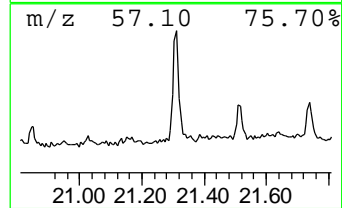
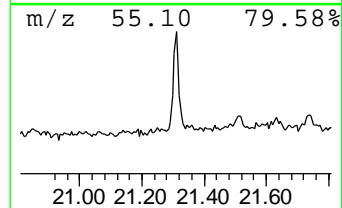
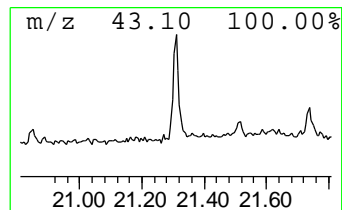
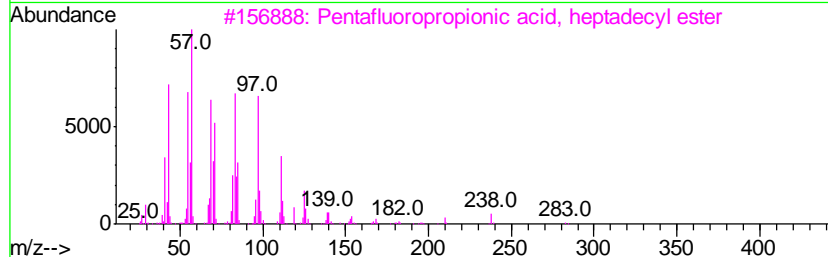
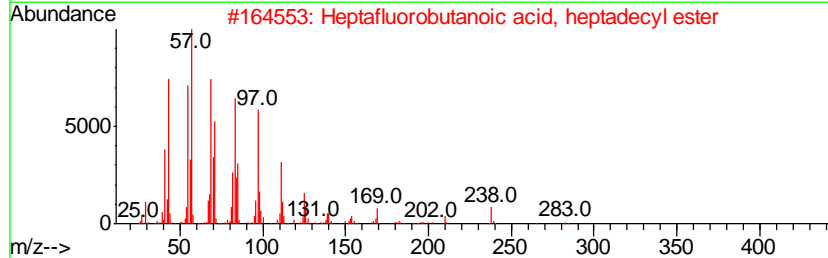
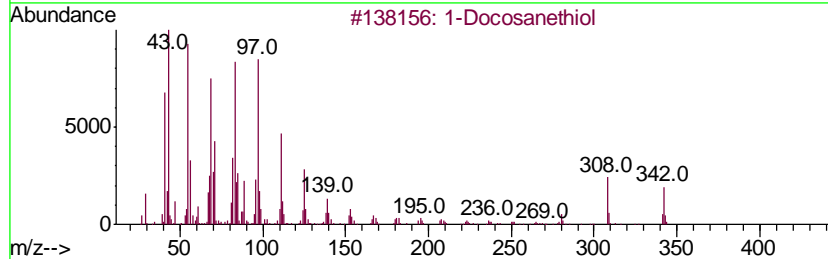
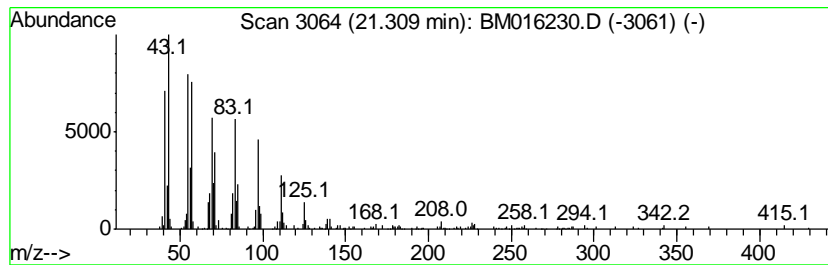
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 Peak Number 6 1-Docosanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	5.02 ng	350844	Chrysene-d12	21.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosanethiol	342	C22H46S	007773-83-3	93
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
4		Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	90
5		17-Pentatriacontene	491	C35H70	006971-40-0	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	9.7	ng	200485	1	8.14	412665	20.0
unknown7.67	7.67	101.9	ng	2101750	1	8.14	412665	20.0
n-Hexadecanoic acid	18.36	10.3	ng	500332	4	17.51	976372	20.0
Octadecanoic acid	19.62	2.5	ng	171300	5	21.64	1398970	20.0
1-Docosanethiol	21.31	5.0	ng	350844	5	21.64	1398970	20.0