

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
 Data File : BM016359.D
 Acq On : 14 Aug 2018 17:49
 Operator : SJ/JU
 Sample : J4443-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SALEM-RD-SP

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	5.169	315	320	331	rVB	127368	189555	9.15%	1.282%
2	5.645	395	401	415	rBV	888938	1326141	64.02%	8.969%
3	7.287	674	680	699	rBV	850018	1403309	67.74%	9.491%
4	7.645	734	741	751	rBV	1002897	1550136	74.83%	10.484%
5	8.116	815	821	831	rVB	195039	309802	14.95%	2.095%
6	8.434	869	875	887	rBB	689866	1106165	53.40%	7.481%
7	9.304	1016	1023	1039	rBV	532898	863067	41.66%	5.837%
8	10.927	1293	1299	1309	rBV	224946	374774	18.09%	2.535%
9	13.374	1708	1715	1725	rBV	1138572	1626049	78.49%	10.997%
10	14.204	1851	1856	1864	rBB	61682	87970	4.25%	0.595%
11	14.751	1943	1949	1957	rVB2	290676	446694	21.56%	3.021%
12	16.245	2197	2203	2215	rBV	1119990	1572629	75.91%	10.636%
13	17.486	2409	2414	2425	rVB2	340565	498348	24.06%	3.370%
14	18.339	2554	2559	2570	rBV2	100347	136839	6.61%	0.925%
15	19.598	2768	2773	2778	rBV3	34763	48032	2.32%	0.325%
16	20.068	2848	2853	2859	rBV	1820570	2071568	100.00%	14.011%
17	21.292	3057	3061	3068	rBV2	74918	126121	6.09%	0.853%
18	21.621	3112	3117	3122	rBV	359289	466600	22.52%	3.156%
19	22.156	3206	3208	3211	rVB2	33050	32754	1.58%	0.222%
20	23.150	3374	3377	3382	rVB	58477	75069	3.62%	0.508%
21	23.950	3507	3513	3522	rVB	236081	474094	22.89%	3.206%

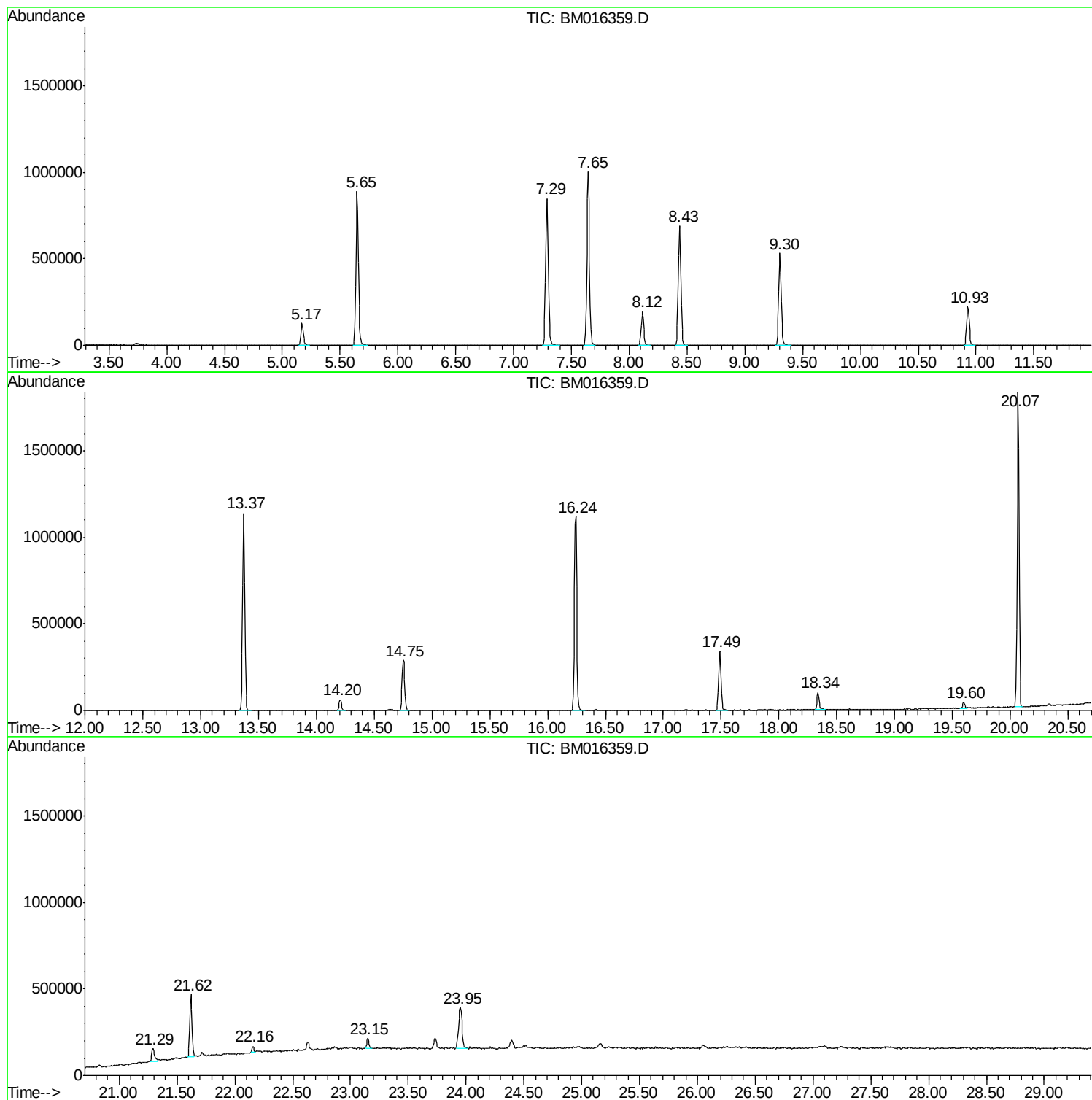
Sum of corrected areas: 14785716

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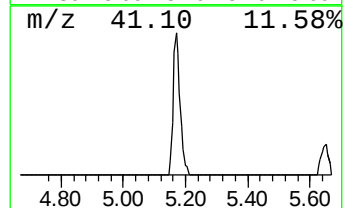
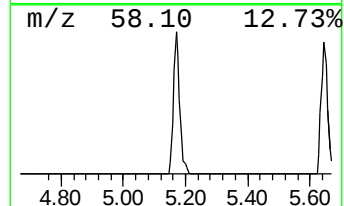
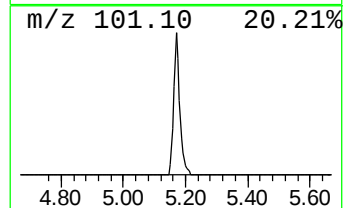
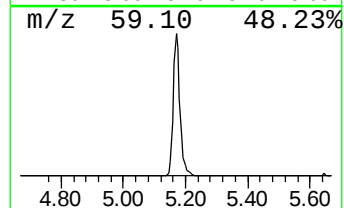
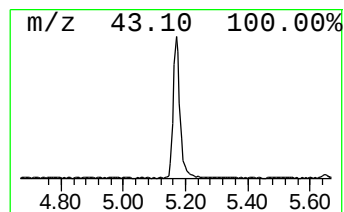
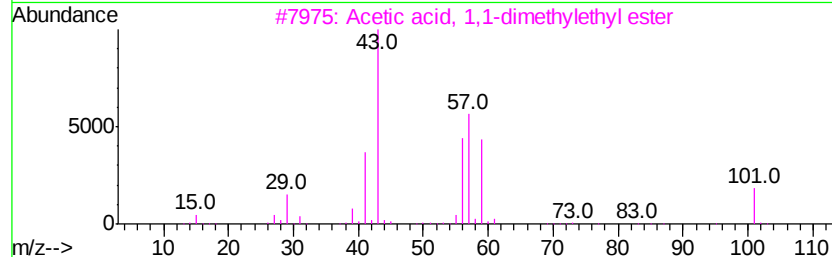
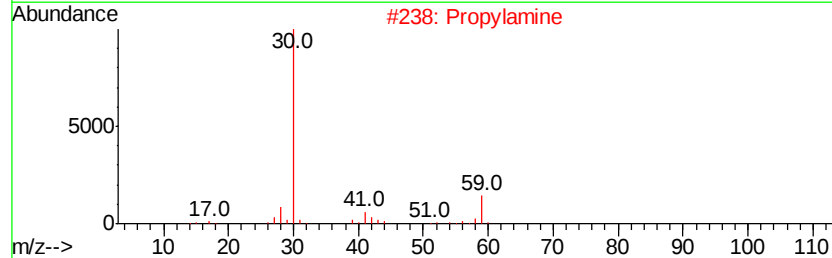
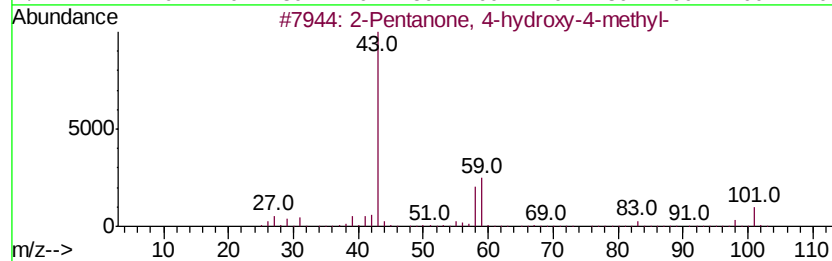
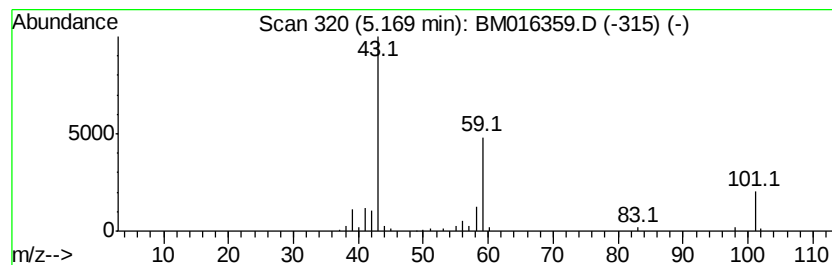
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	12.24 ng	189555	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Propylamine	59	C3H9N	000107-10-8	38
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
5		Butane	58	C4H10	000106-97-8	22



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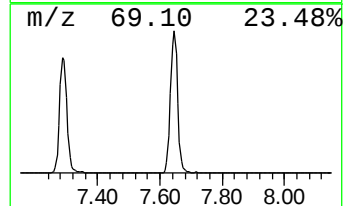
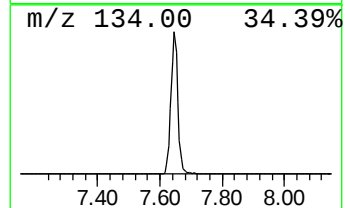
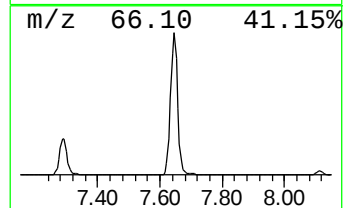
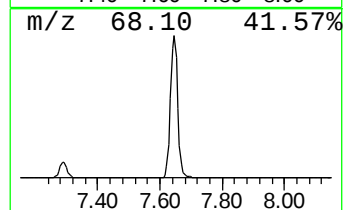
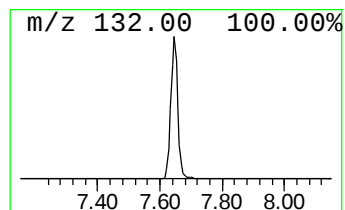
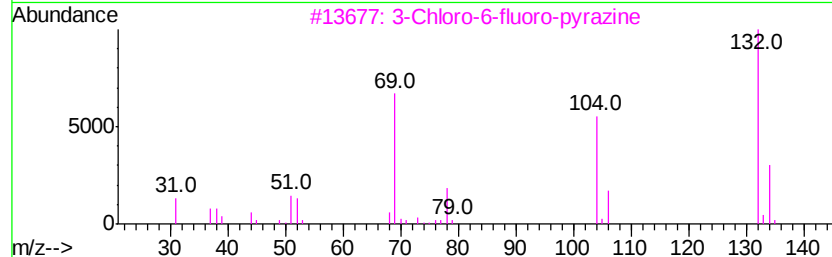
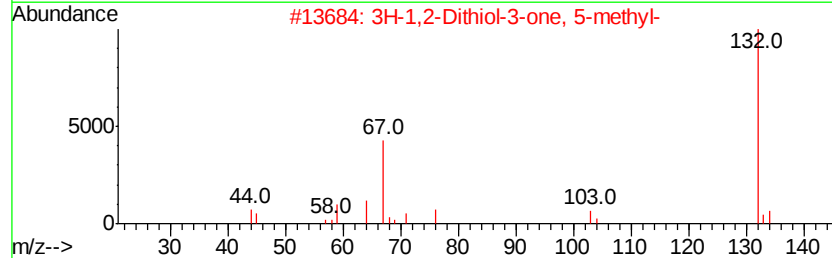
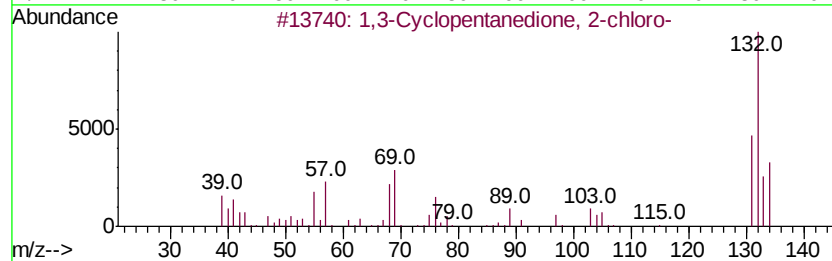
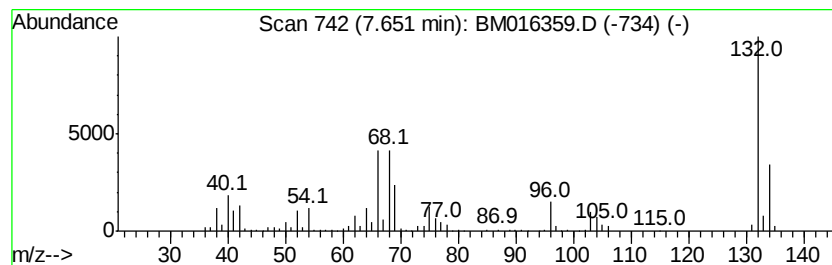
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Peak Number 2 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	100.07 ng	1550140	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14



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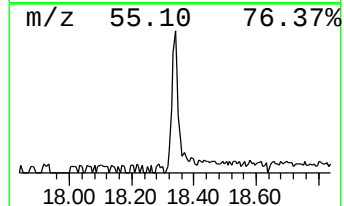
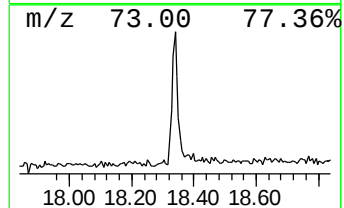
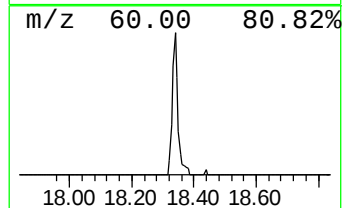
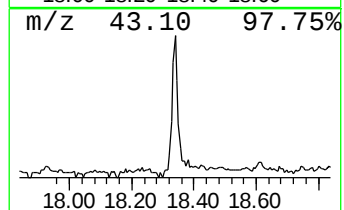
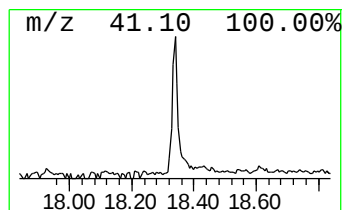
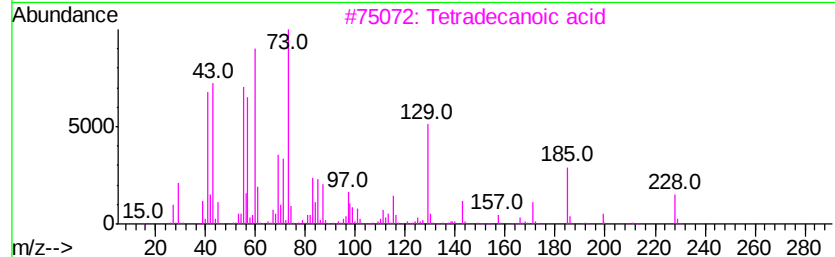
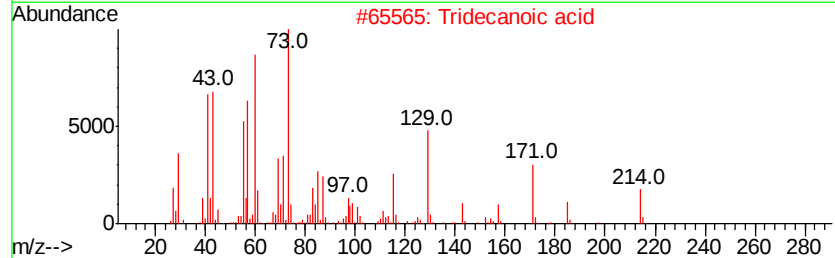
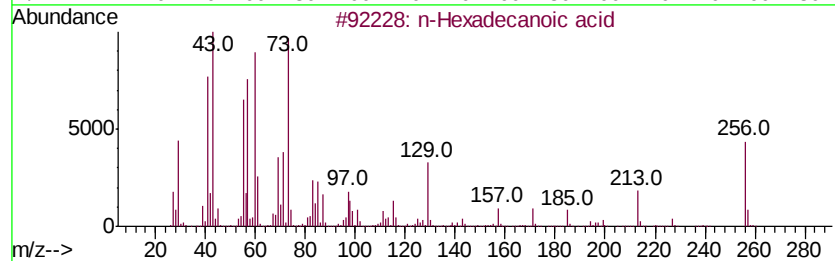
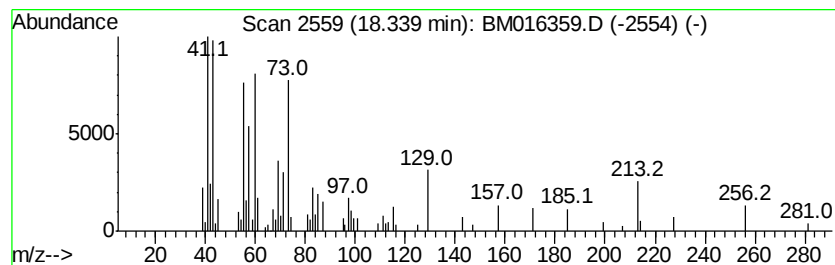
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	5.49 ng	136839	Phenanthrene-d10	17.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5		n-Decanoic acid	172	C10H20O2	000334-48-5	49



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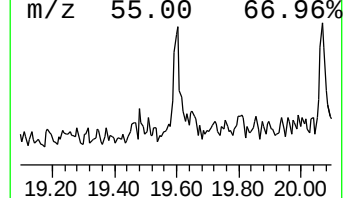
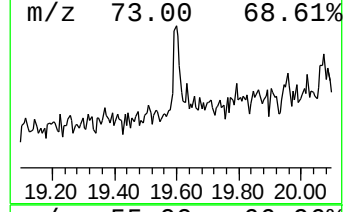
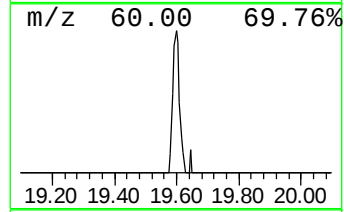
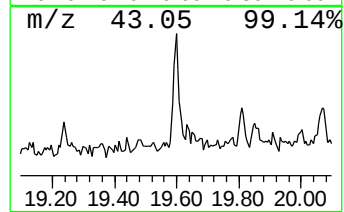
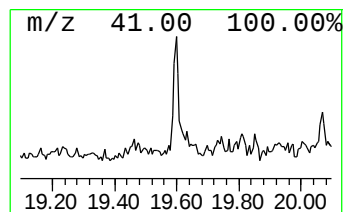
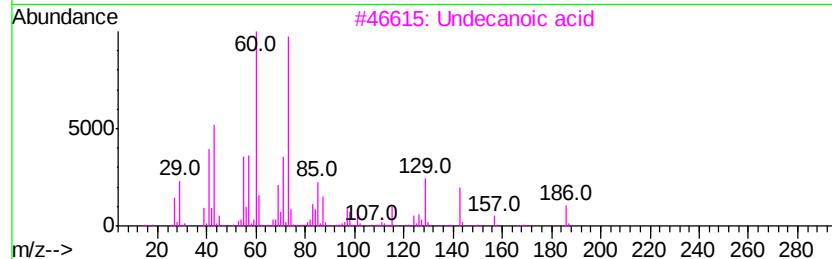
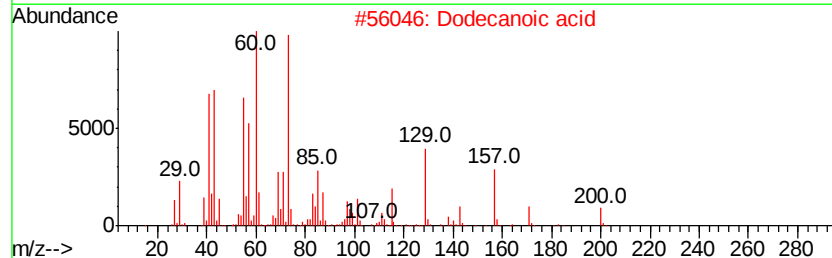
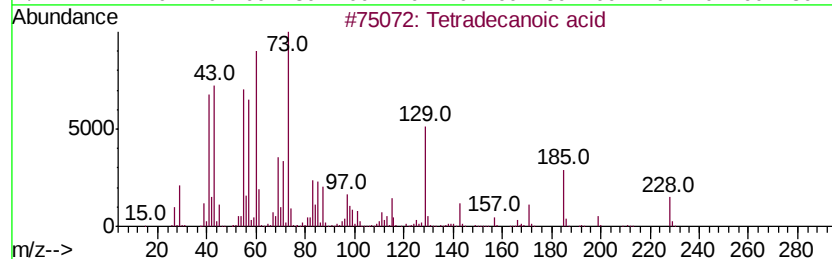
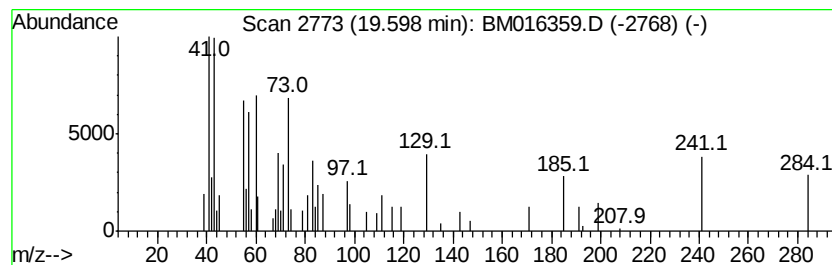
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Peak Number 5 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.60	2.06 ng	48032	Chrysene-d12	21.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
2		Dodecanoic acid	200	C12H24O2	000143-07-7	27
3		Undecanoic acid	186	C11H22O2	000112-37-8	27
4		n-Decanoic acid	172	C10H20O2	000334-48-5	22
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	22



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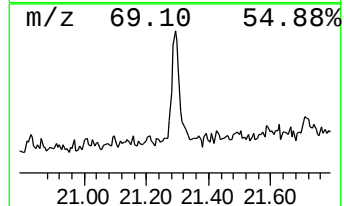
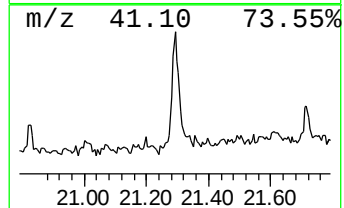
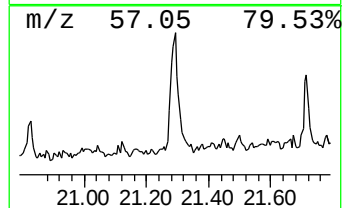
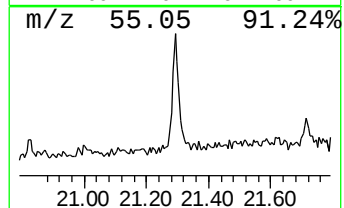
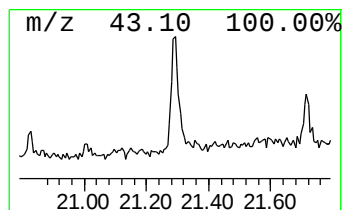
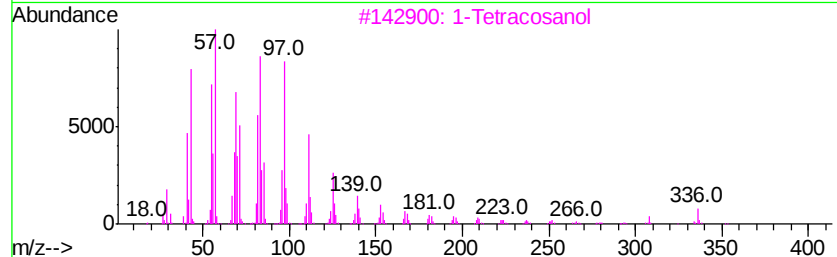
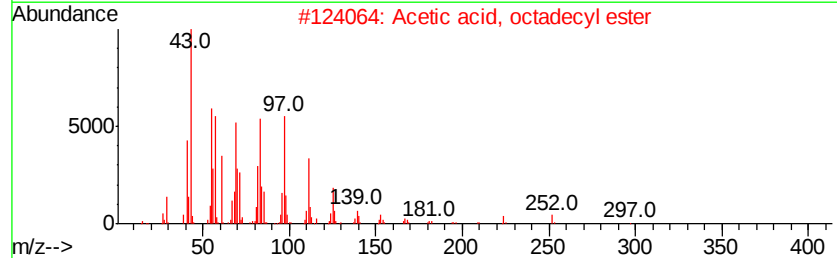
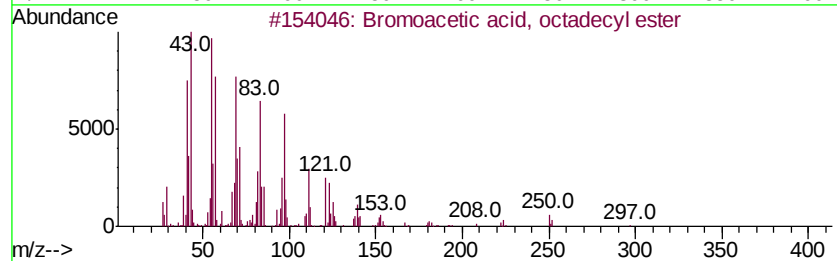
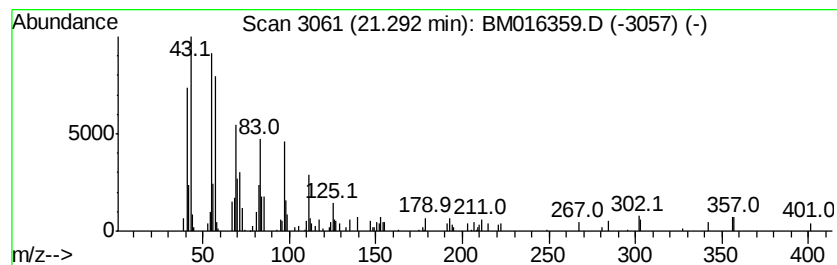
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Bromoacetic acid, octadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.29	5.41 ng	126121	Chrysene-d12	21.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	89
2	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	76
3	1-Tetracosanol	354	C24H50O	000506-51-4	76
4	1-Docosanethiol	342	C22H46S	007773-83-3	70
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	68



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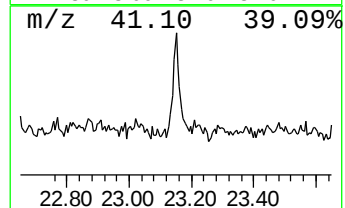
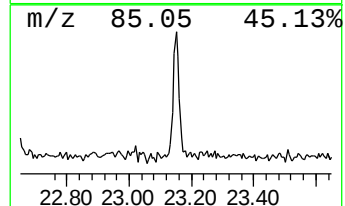
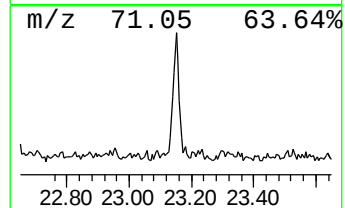
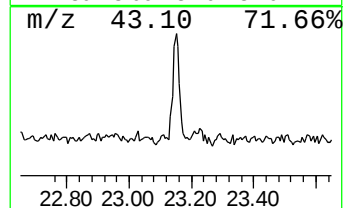
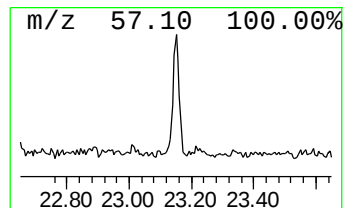
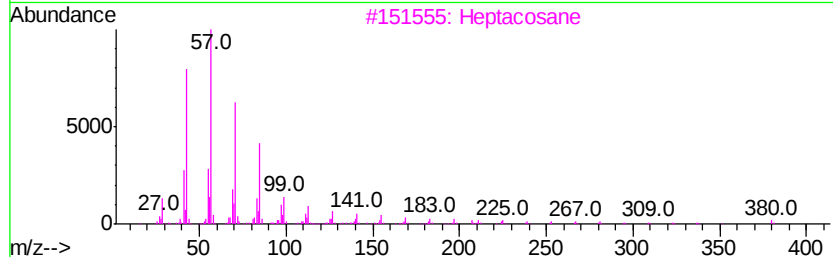
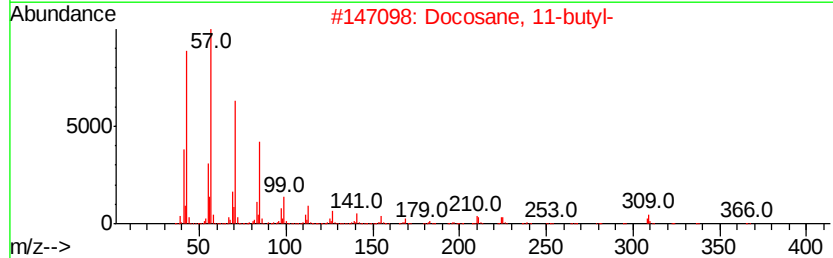
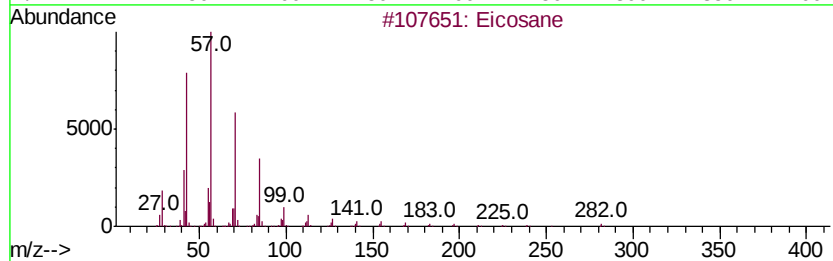
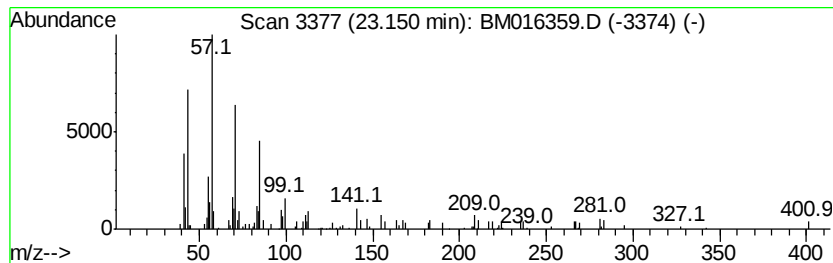
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	3.17 ng	75069	Perylene-d12	23.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	92
2	Docosane, 11-butyl-		366	C26H54	013475-76-8	81
3	Heptacosane		380	C27H56	000593-49-7	76
4	Tetratriacontane		479	C34H70	014167-59-0	70
5	10-Methylnonadecane		282	C20H42	056862-62-5	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM081418\
Data File : BM016359.D
Acq On : 14 Aug 2018 17:49
Operator : SJ/JU
Sample : J4443-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SALEM-RD-SP

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	12.2	ng	189555	1	8.12	309802	20.0
unknown7.65	7.65	100.1	ng	1550140	1	8.12	309802	20.0
n-Hexadecanoic acid	18.34	5.5	ng	136839	4	17.49	498348	20.0
Tetradecanoic acid	19.60	2.1	ng	48032	5	21.62	466600	20.0
Bromoacetic acid,...	21.29	5.4	ng	126121	5	21.62	466600	20.0
Eicosane	23.15	3.2	ng	75069	6	23.95	474094	20.0