

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
 Data File : BM016360.D
 Acq On : 14 Aug 2018 18:26
 Operator : SJ/JU
 Sample : J4459-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FRAC-TANK-SV30518L

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	rBV	63680	93562	2.98%	0.591%
2	5.646	395	401	419	rBV	481237	741060	23.62%	4.682%
3	7.287	674	680	701	rBB	271110	456109	14.54%	2.882%
4	7.645	734	741	756	rBV	1015631	1582403	50.44%	9.999%
5	8.116	815	821	830	rBB	179221	286576	9.13%	1.811%
6	8.434	868	875	888	rBB	893567	1432061	45.64%	9.049%
7	9.304	1016	1023	1038	rBV	674133	1106833	35.28%	6.994%
8	10.928	1293	1299	1308	rBV	207708	337586	10.76%	2.133%
9	13.374	1708	1715	1726	rVB	1649935	2338479	74.54%	14.776%
10	14.204	1852	1856	1862	rBV	58890	79581	2.54%	0.503%
11	14.751	1943	1949	1958	rVB2	283599	405097	12.91%	2.560%
12	16.245	2196	2203	2211	rBV	1547940	2082631	66.38%	13.159%
13	17.486	2409	2414	2421	rBV2	316499	446790	14.24%	2.823%
14	18.339	2555	2559	2565	rBV	118550	162739	5.19%	1.028%
15	19.533	2758	2762	2767	rVB	74446	91599	2.92%	0.579%
16	19.598	2769	2773	2783	rBV2	68358	104961	3.35%	0.663%
17	20.068	2848	2853	2859	rBV	2713284	3137400	100.00%	19.824%
18	20.827	2978	2982	2987	rBV3	30300	47056	1.50%	0.297%
19	21.292	3057	3061	3068	rBV8	31214	56361	1.80%	0.356%
20	21.621	3112	3117	3123	rBV	330348	413211	13.17%	2.611%
21	23.950	3507	3513	3520	rVB2	220443	424212	13.52%	2.680%

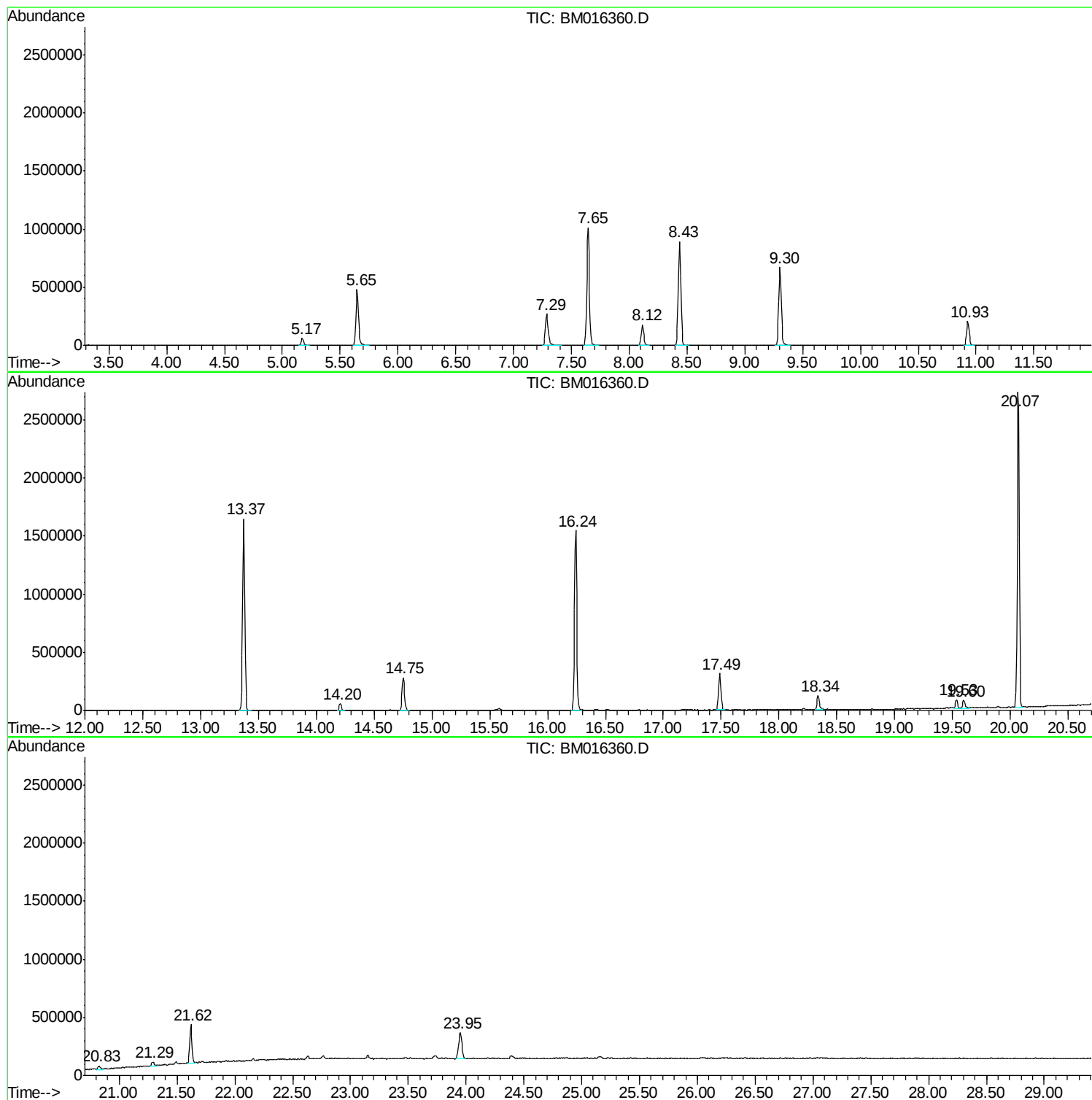
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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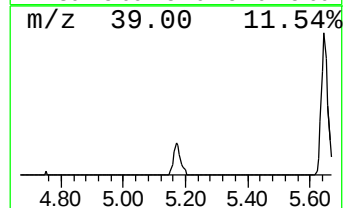
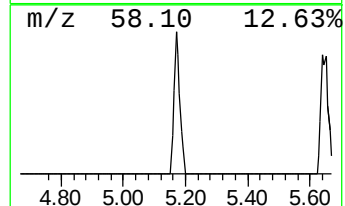
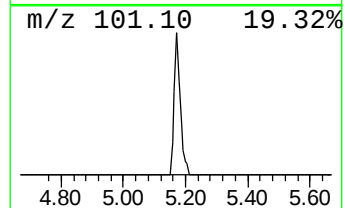
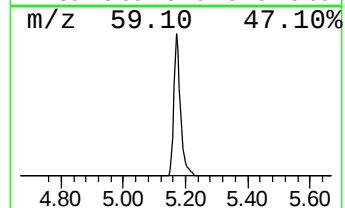
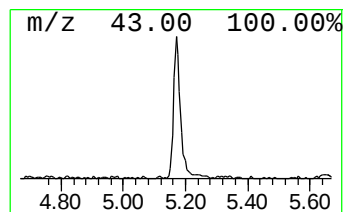
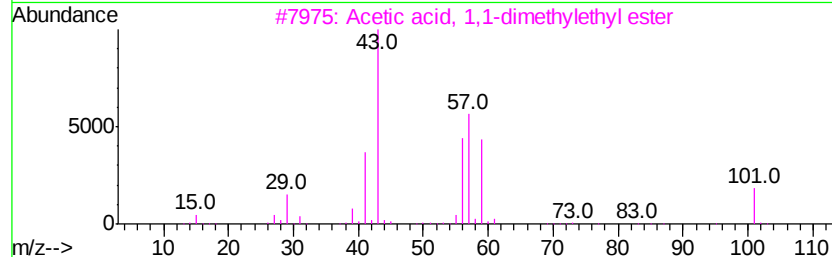
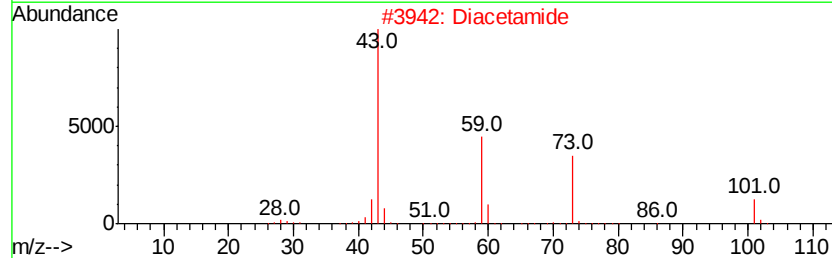
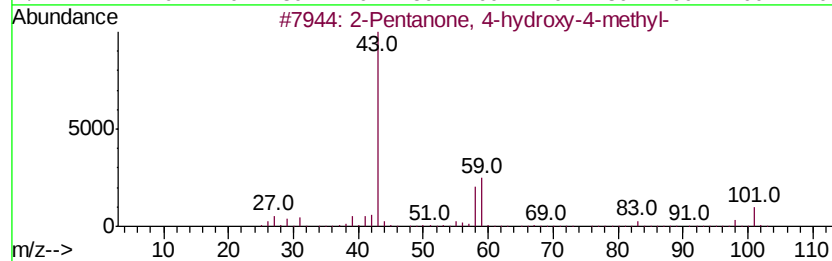
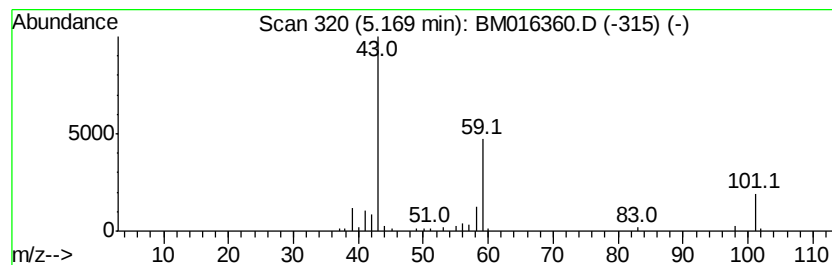
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	6.53 ng	93562	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Diacetamide	101	C4H7NO2	000625-77-4	64
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
5			Butane	58	C4H10	000106-97-8	10



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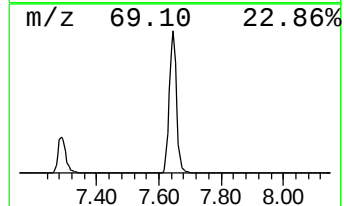
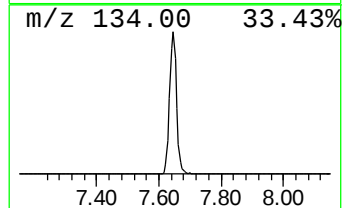
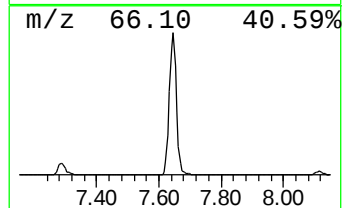
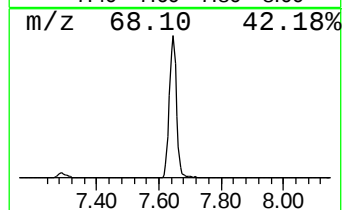
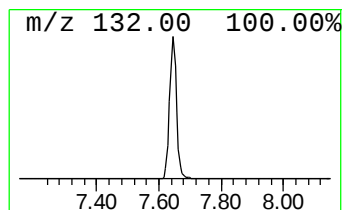
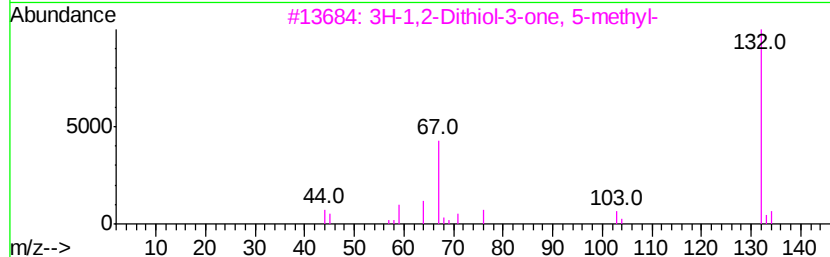
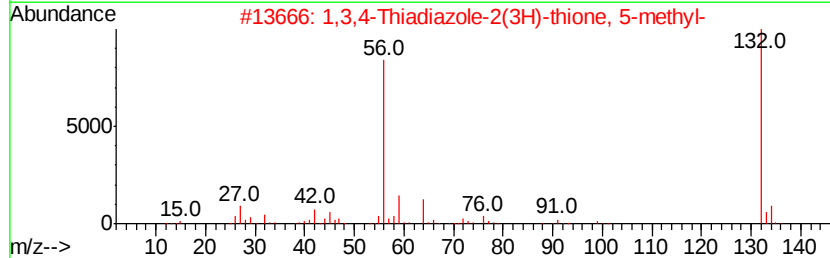
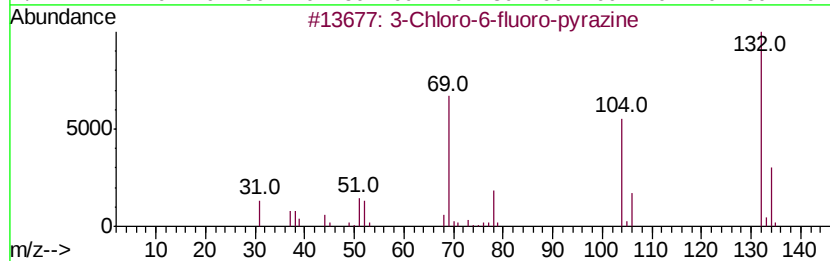
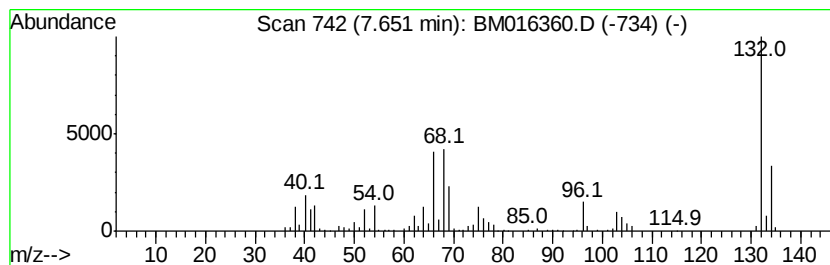
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	110.44 ng	1582400	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	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-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12



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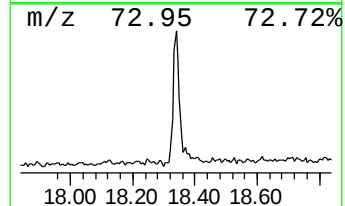
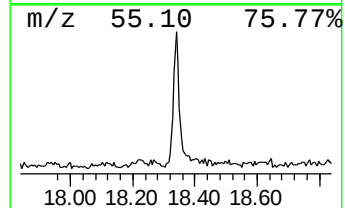
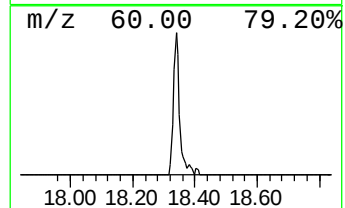
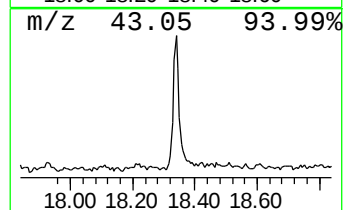
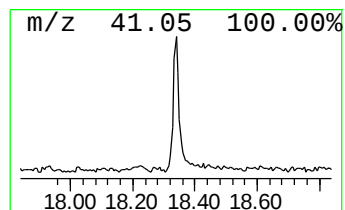
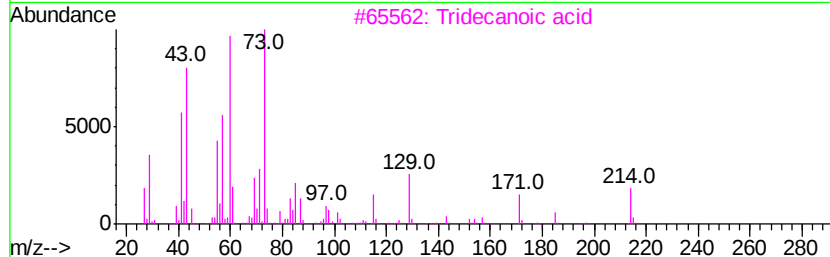
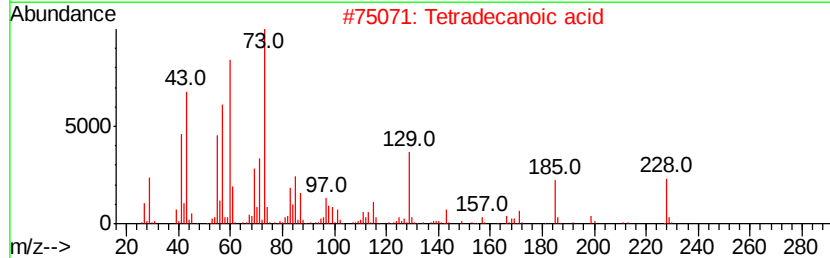
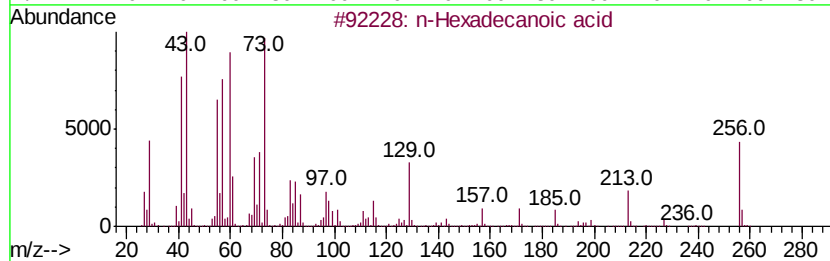
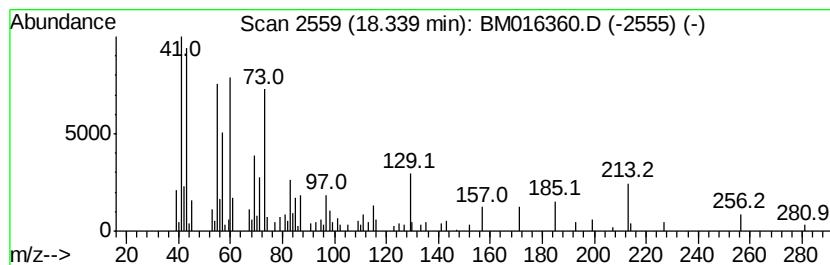
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	7.28 ng	162739	Phenanthrene-d10	17.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Tridecanoic acid	214	C13H26O2	000638-53-9	58
4	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49



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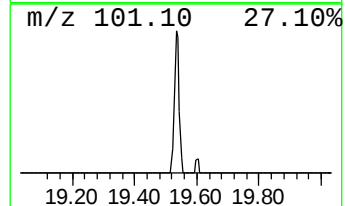
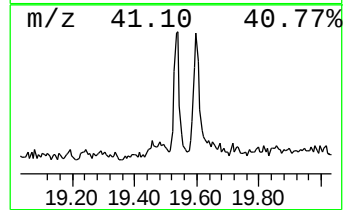
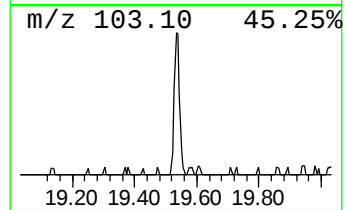
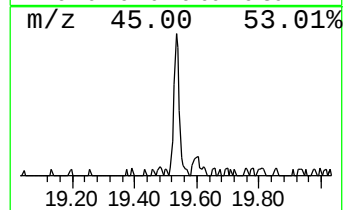
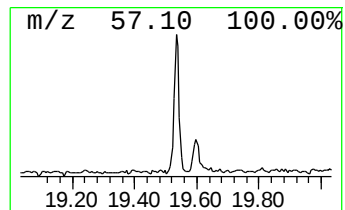
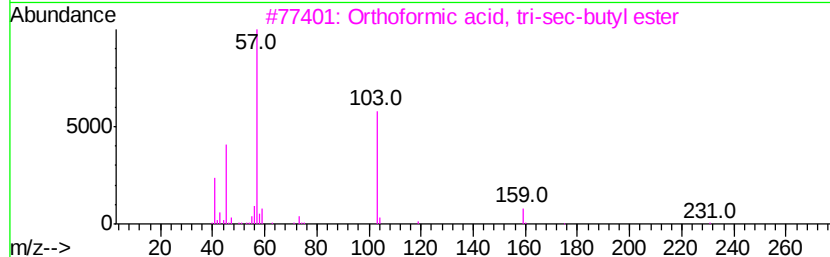
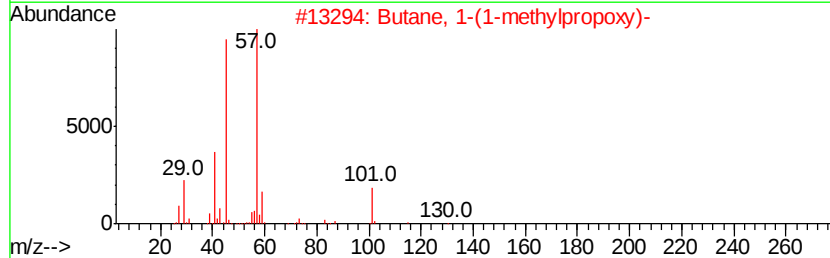
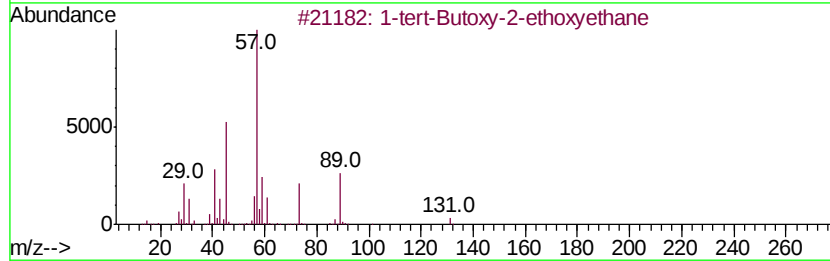
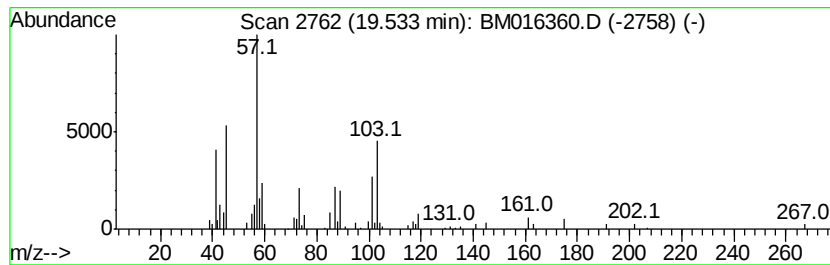
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Peak Number 5 unknown19.53 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.53	4.10 ng	91599	Phenanthrene-d10	17.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	43
2		Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	38
3		Orthoformic acid, tri-sec-butyl ...	232	C13H28O3	016754-48-6	38
4		Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	37
5		Butane, 1,2,4-trimethoxy-	148	C7H16O3	020637-48-3	32



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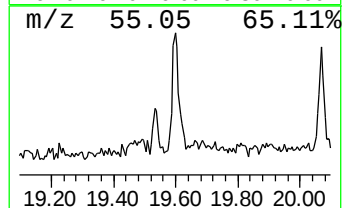
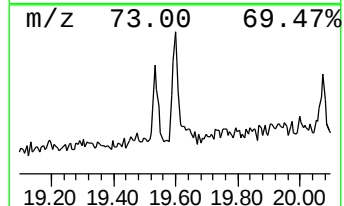
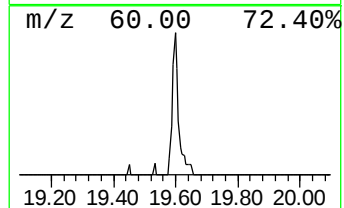
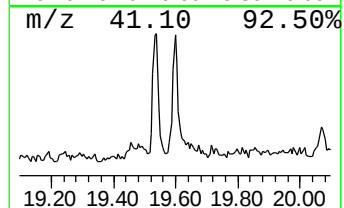
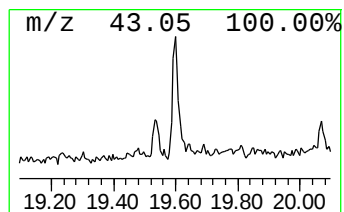
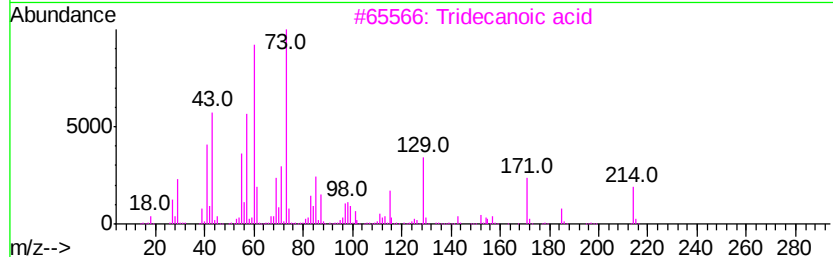
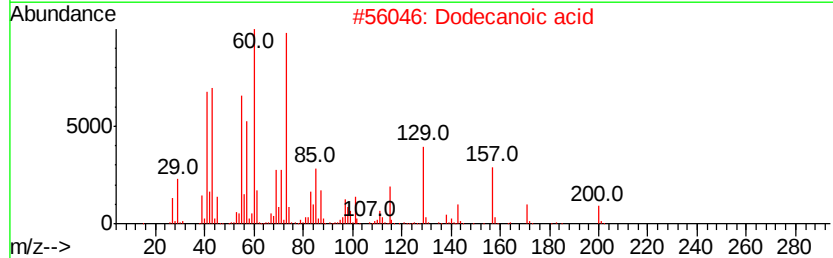
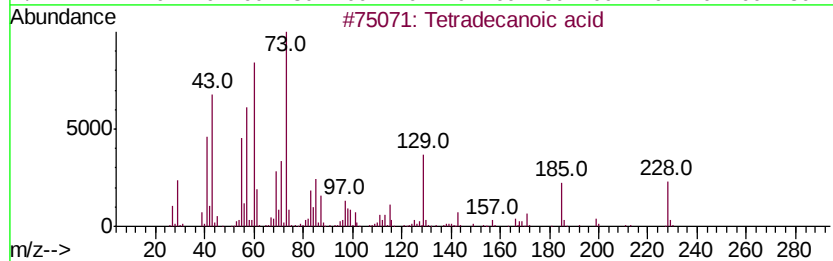
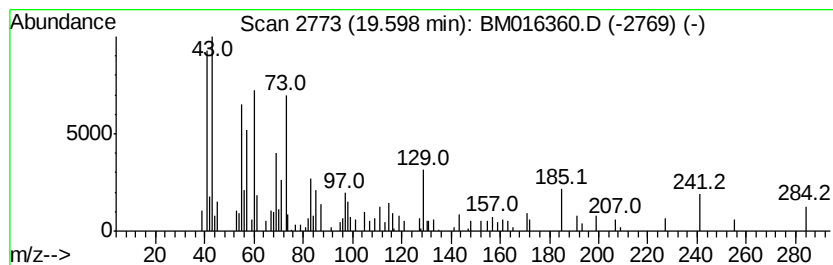
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.60	5.08 ng	104961	Chrysene-d12	21.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
2		Dodecanoic acid	200	C12H24O2	000143-07-7	46
3		Tridecanoic acid	214	C13H26O2	000638-53-9	43
4		n-Decanoic acid	172	C10H20O2	000334-48-5	38
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	35



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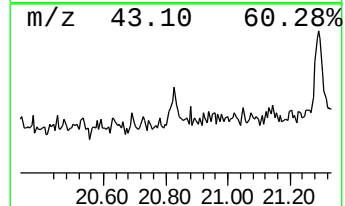
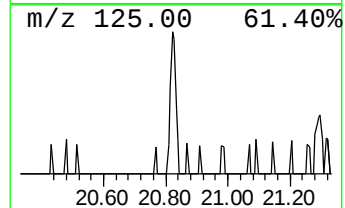
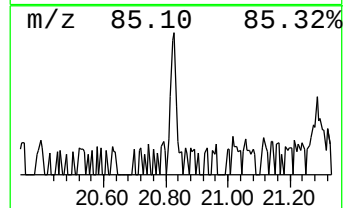
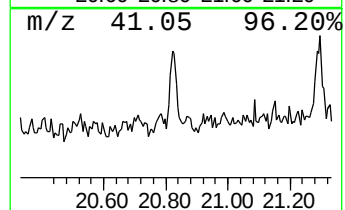
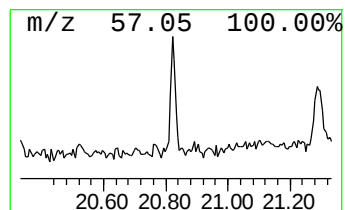
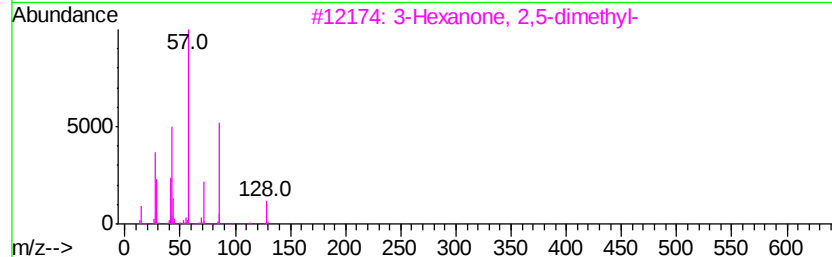
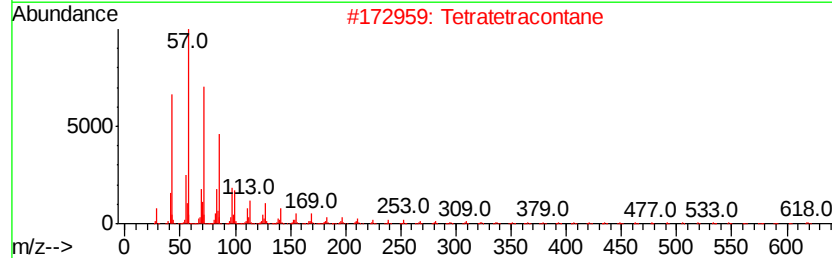
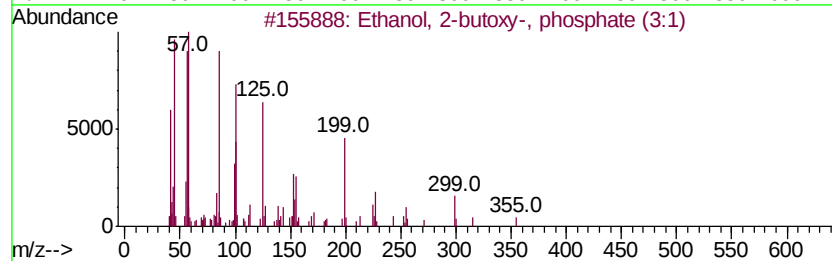
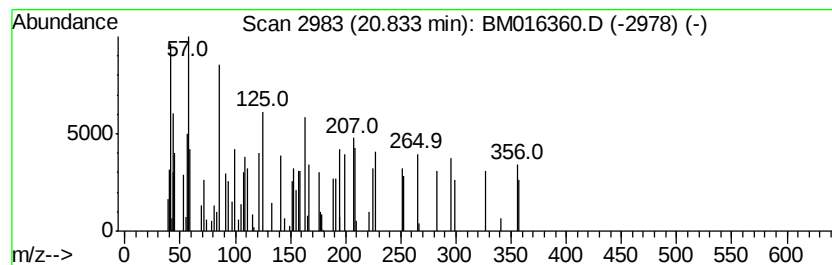
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Ethanol, 2-butoxy-, phospho... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.83	2.28 ng	47056	Chrysene-d12	21.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	50
2		Tetratetracontane	619	C44H90	007098-22-8	14
3		3-Hexanone, 2,5-dimethyl-	128	C8H16O	001888-57-9	11
4		Isobutyl 3-hydroxy-2-methylenebu...	172	C9H16O3	080758-68-5	10
5		5-Nitrofuran-2-carboxaldehyde va...	239	C10H13N3O4	1000252-69-8	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081418\
Data File : BM016360.D
Acq On : 14 Aug 2018 18:26
Operator : SJ/JU
Sample : J4459-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

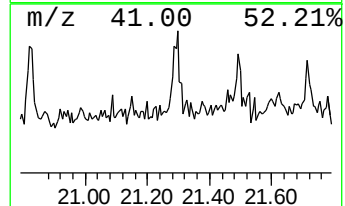
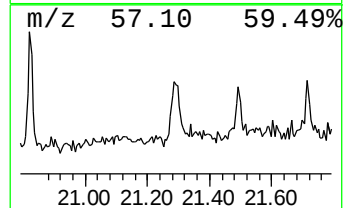
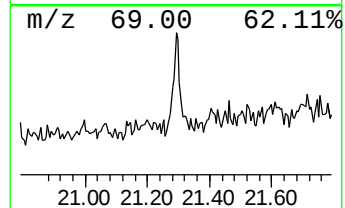
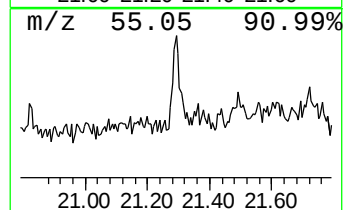
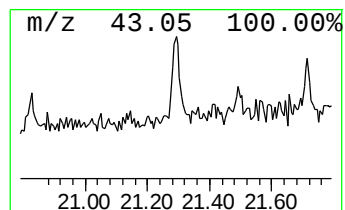
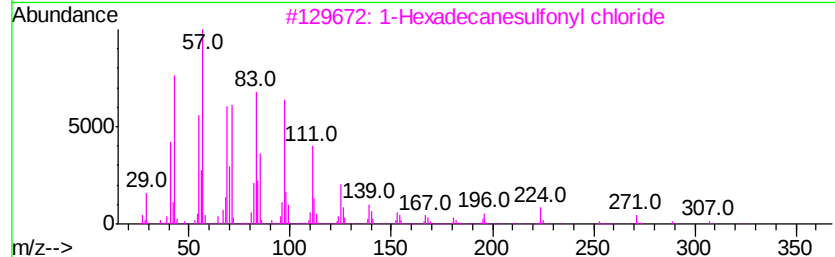
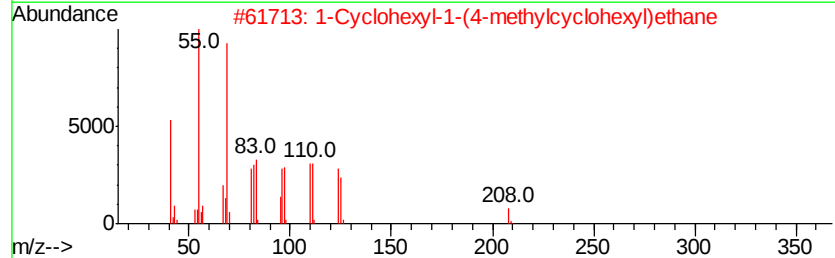
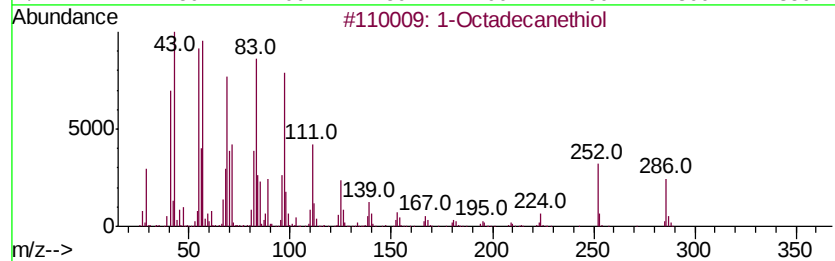
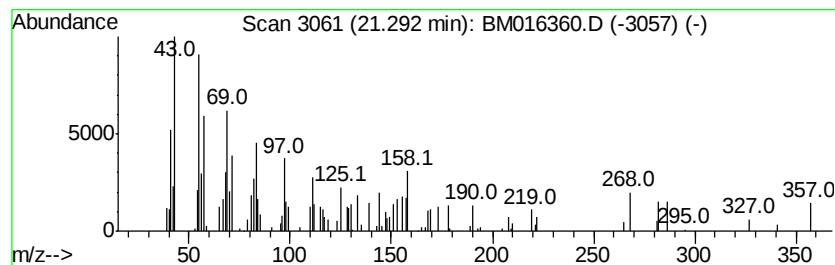
Instrument :
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ClientSampleId :
FRAC-TANK-SV30518L

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 8 unknown21.29 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	2.73 ng	56361	Chrysene-d12	21.62
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Octadecanethiol	286	C18H38S	002885-00-9 43
2	1-Cyclohexyl-1-(4-methylcyclohex...	208	C15H28	002027-12-5 38
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1 35
4	4-Chloro-3-n-hexyltetrahydropyran	204	C11H21ClO	066555-66-6 27
5	Pentadec-7-ene, 7-bromomethyl-	302	C16H31Br	1000259-58-5 25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM081418\
Data File : BM016360.D
Acq On : 14 Aug 2018 18:26
Operator : SJ/JU
Sample : J4459-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FRAC-TANK-SV30518L

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	6.5	ng	93562	1	8.12	286576	20.0
unknown7.65	7.65	110.4	ng	1582400	1	8.12	286576	20.0
n-Hexadecanoic acid	18.34	7.3	ng	162739	4	17.49	446790	20.0
unknown19.53	19.53	4.1	ng	91599	4	17.49	446790	20.0
Tetradecanoic acid	19.60	5.1	ng	104961	5	21.62	413211	20.0
Ethanol, 2-butoxy...	20.83	2.3	ng	47056	5	21.62	413211	20.0
unknown21.29	21.29	2.7	ng	56361	5	21.62	413211	20.0