

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121618\
 Data File : BM018238.D
 Acq On : 16 Dec 2018 22:12
 Operator : JU/SJ
 Sample : J6386-08
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P001-SS005-1824-01

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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	3.363	77	81	94	rBV	88398	121053	2.09%	0.264%
2	4.687	301	306	315	rBV	101707	147524	2.55%	0.322%
3	5.128	375	381	394	rBV	3017618	4227241	73.10%	9.218%
4	6.698	641	648	662	rBV	2703644	4544053	78.58%	9.909%
5	7.040	698	706	717	rBV	3244189	4971632	85.97%	10.842%
6	7.492	774	783	792	rBV	535114	856621	14.81%	1.868%
7	7.810	830	837	846	rBV	2201084	3376378	58.39%	7.363%
8	8.657	971	981	998	rBV	1749522	2887463	49.93%	6.297%
9	10.263	1246	1254	1271	rBV	643950	1153860	19.95%	2.516%
10	12.763	1672	1679	1692	rBV	3658894	5487957	94.90%	11.968%
11	13.627	1820	1826	1840	rBV	351588	570598	9.87%	1.244%
12	14.157	1909	1916	1930	rVB2	849666	1340333	23.18%	2.923%
13	15.663	2165	2172	2184	rBV	3211846	4531122	78.35%	9.881%
14	16.915	2379	2385	2399	rBV	990348	1493936	25.83%	3.258%
15	17.833	2535	2541	2552	rBV2	309938	522224	9.03%	1.139%
16	19.127	2756	2761	2768	rBV3	87797	163763	2.83%	0.357%
17	19.568	2830	2836	2846	rBV	4636870	5782909	100.00%	12.611%
18	20.856	3051	3055	3062	rBV	450037	629971	10.89%	1.374%
19	21.139	3097	3103	3113	rBV	982321	1496360	25.88%	3.263%
20	21.297	3127	3130	3135	rBV3	53384	67148	1.16%	0.146%
21	22.162	3275	3277	3284	rVB6	78840	101838	1.76%	0.222%
22	23.297	3464	3470	3482	rVB	700707	1382195	23.90%	3.014%

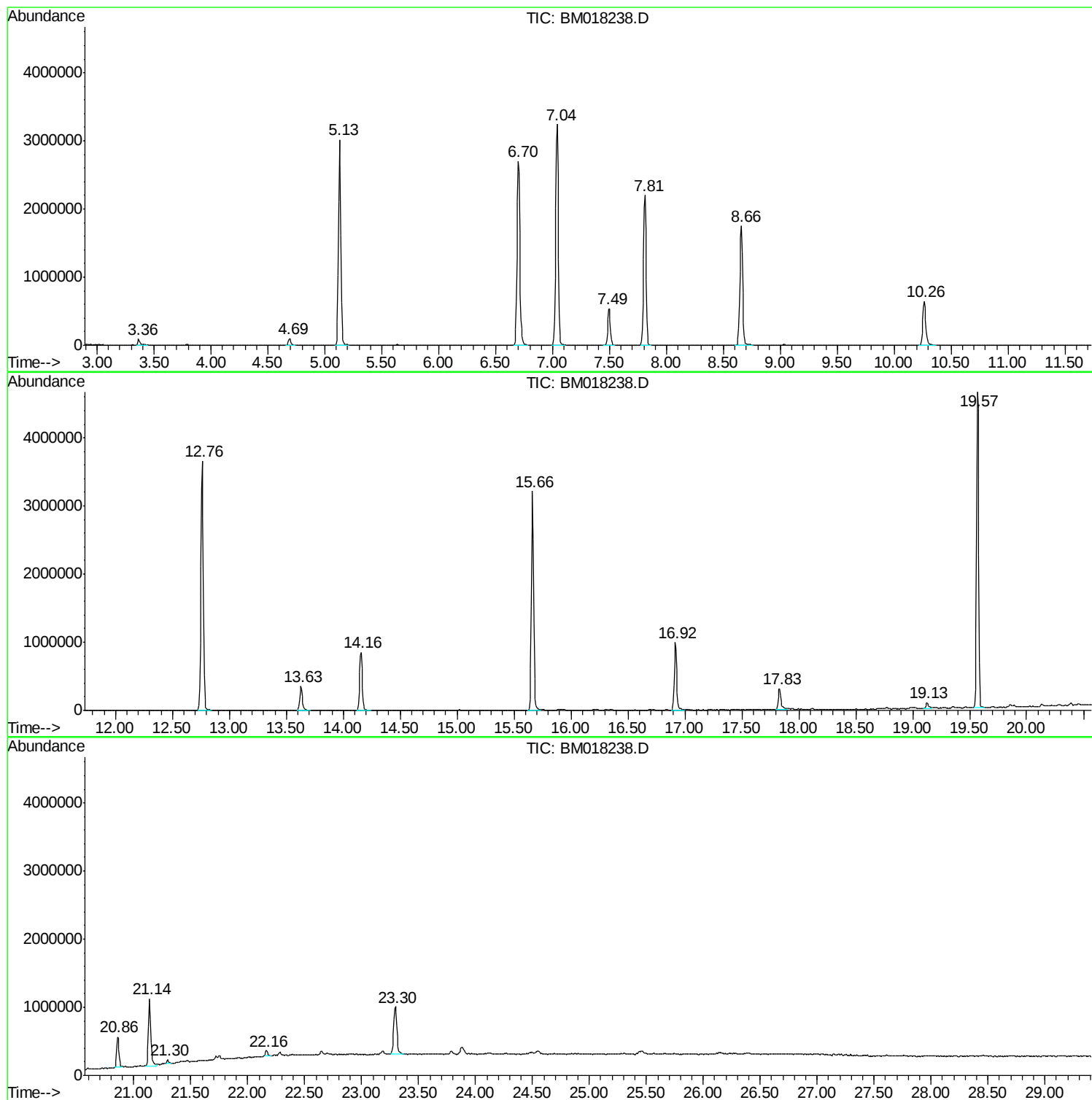
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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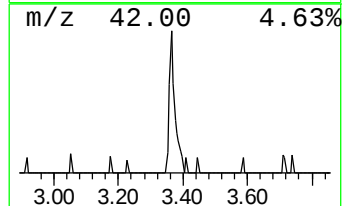
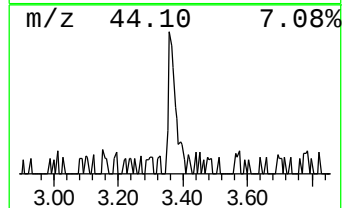
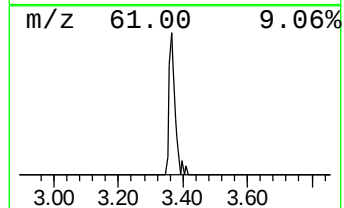
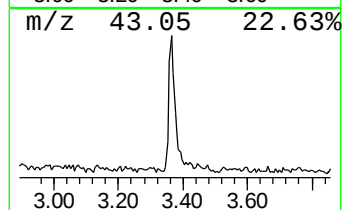
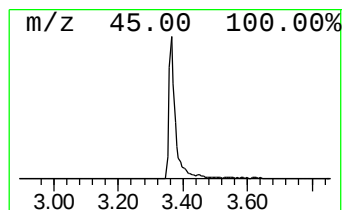
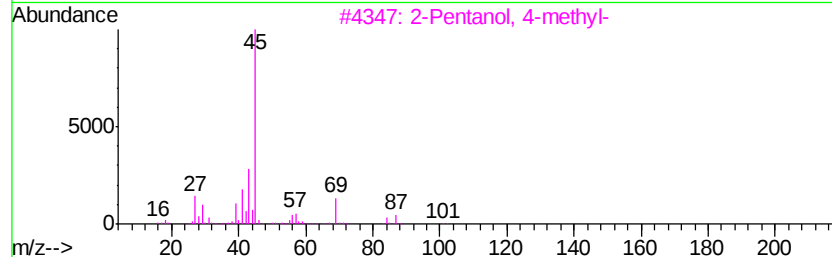
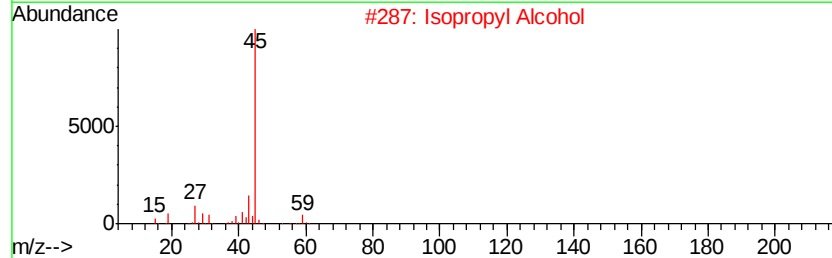
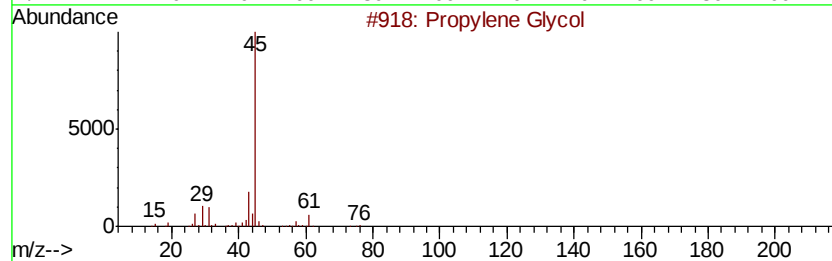
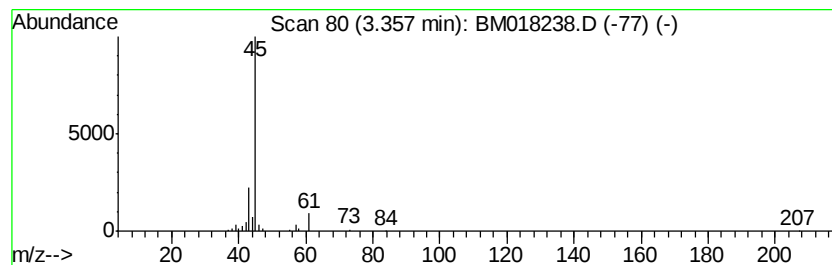
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM121518.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.36	2.83 ng	121053	1,4-Dichlorobenzene-d4	7.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	64
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	64
3		2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	23
4		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
5		2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	9



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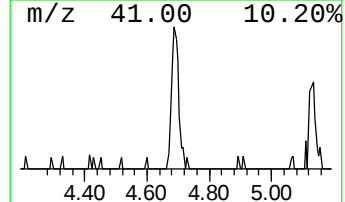
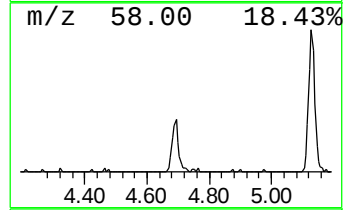
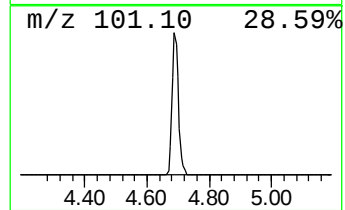
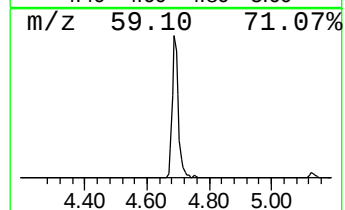
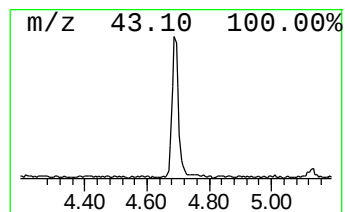
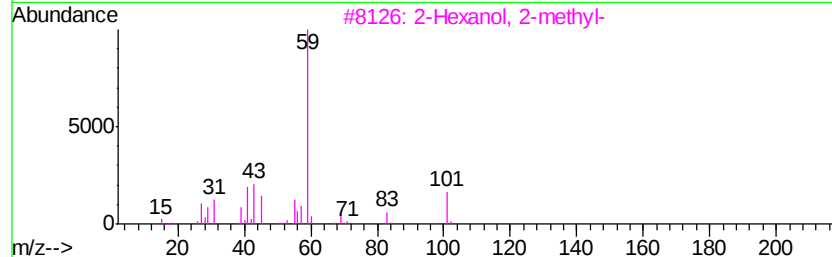
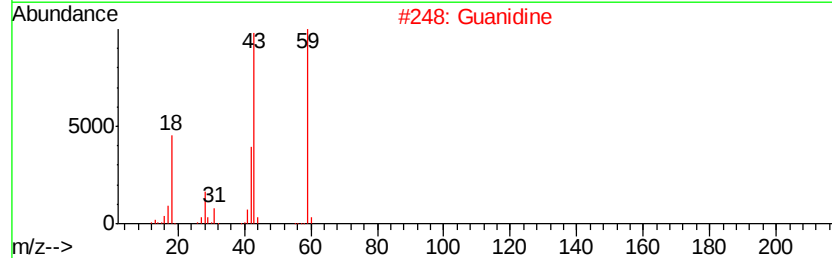
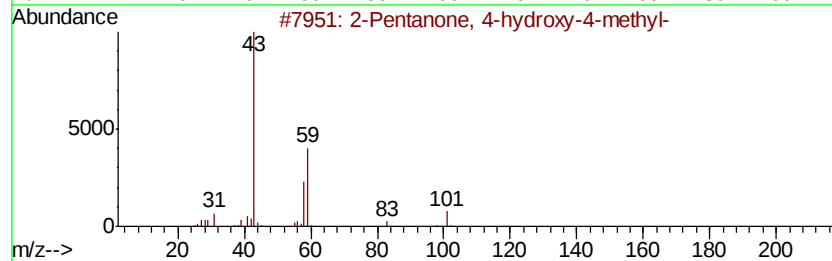
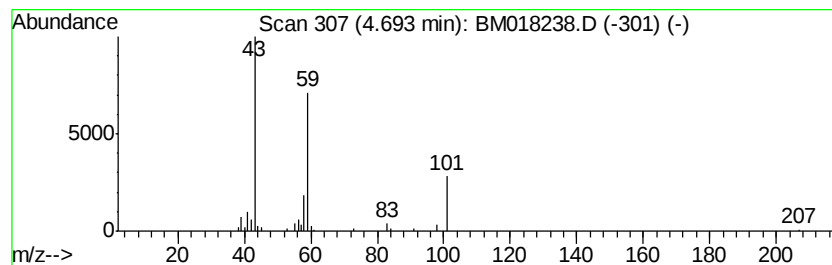
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.69	3.44 ng	147524	1,4-Dichlorobenzene-d4	7.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Guanidine	59	CH5N3	000113-00-8	50
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	45
4	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	38
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	37



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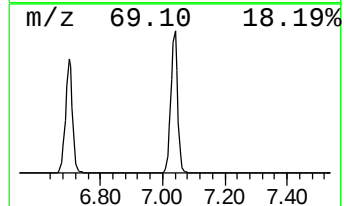
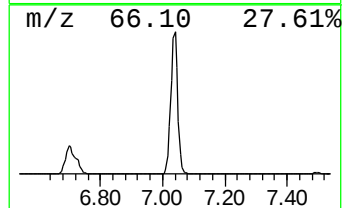
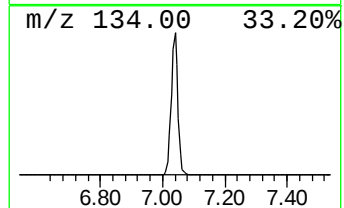
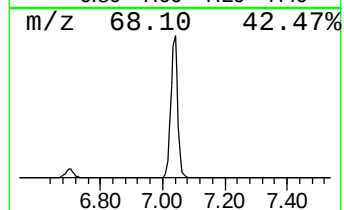
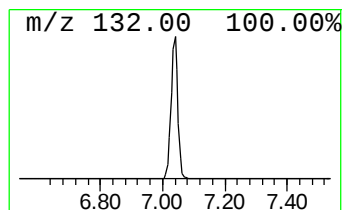
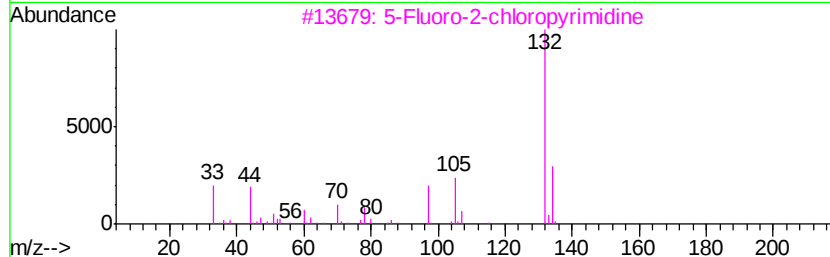
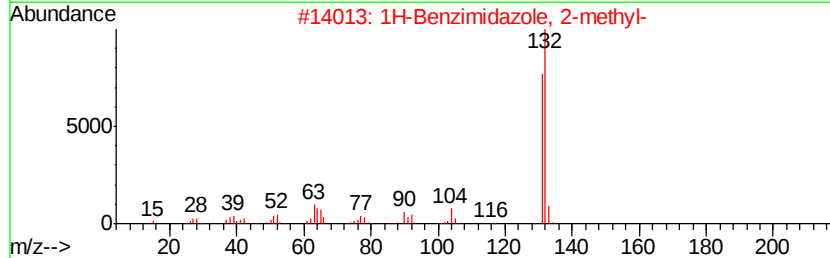
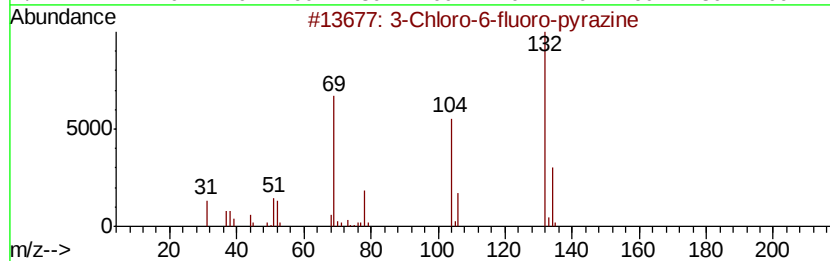
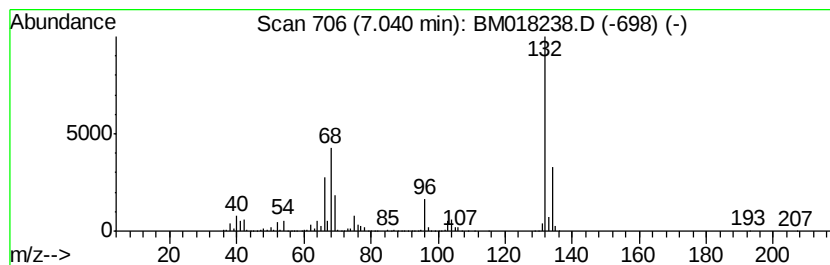
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Peak Number 3 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	116.08 ng	4971630	1,4-Dichlorobenzene-d4	7.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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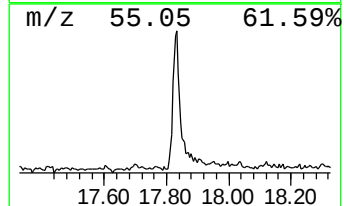
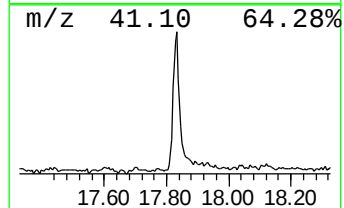
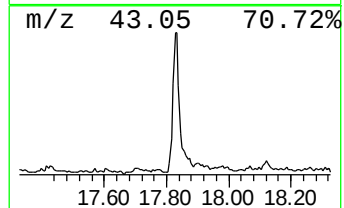
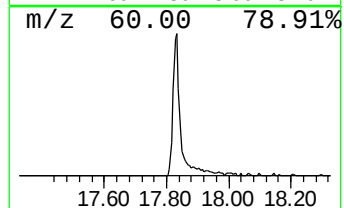
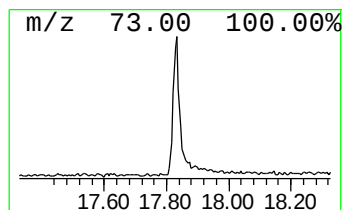
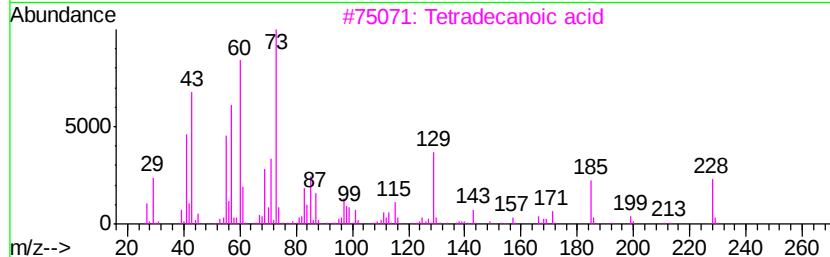
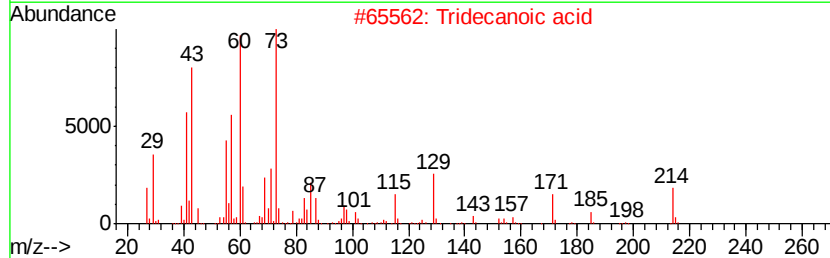
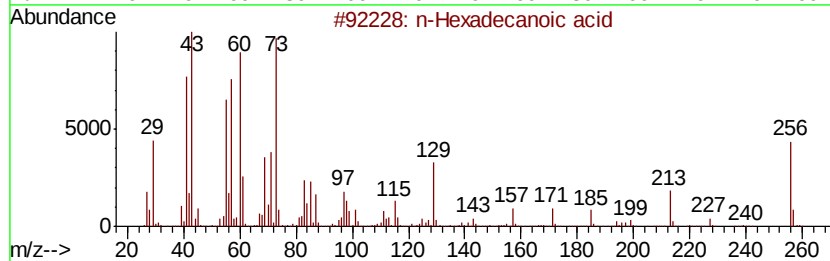
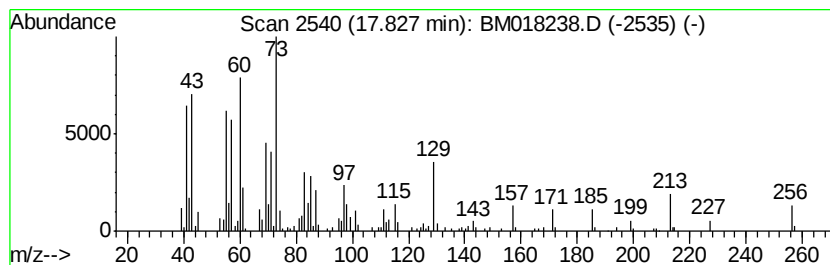
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	6.99 ng	522224	Phenanthrene-d10	16.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5		Dodecanoic acid	200	C12H24O2	000143-07-7	50



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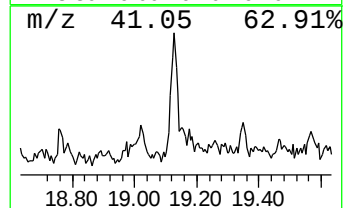
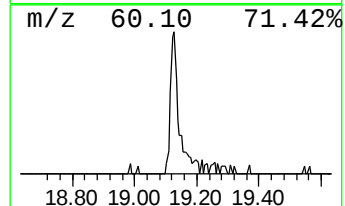
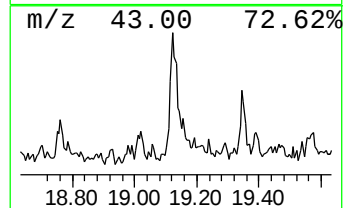
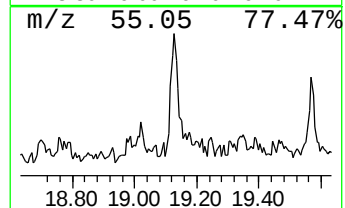
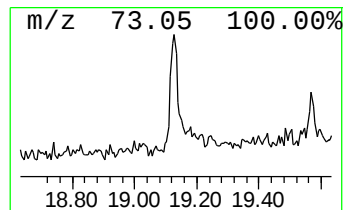
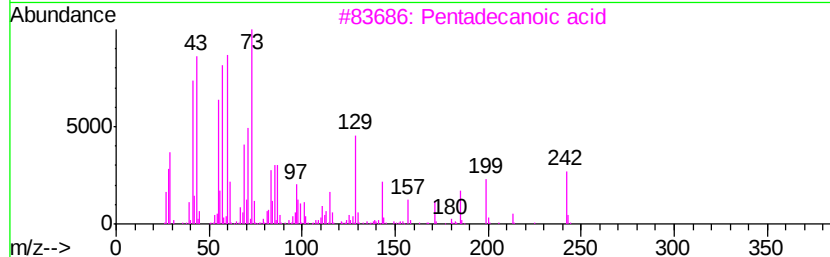
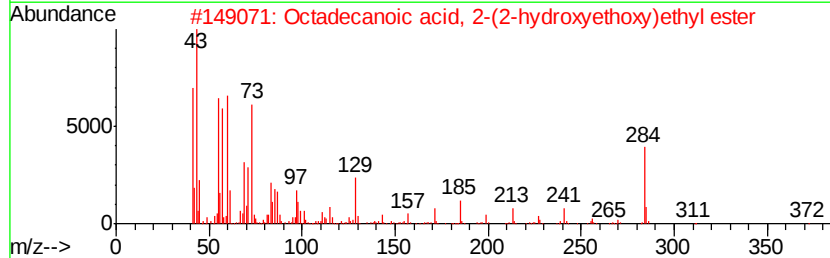
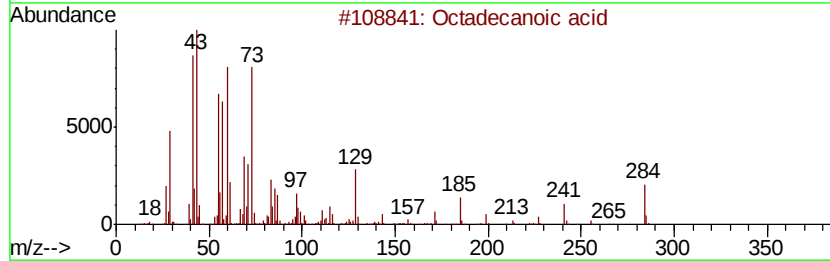
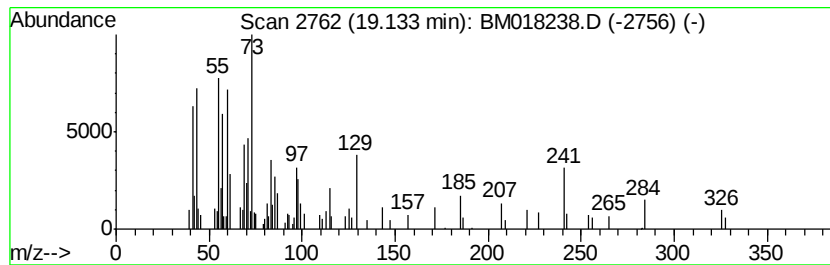
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Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.13	2.19 ng	163763	Chrysene-d12	21.14	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53



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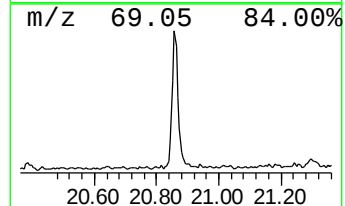
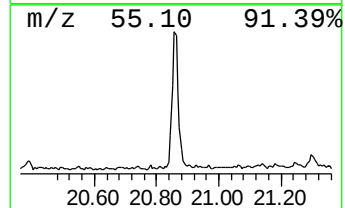
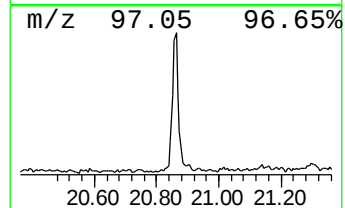
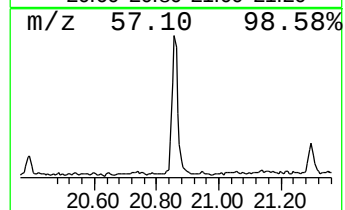
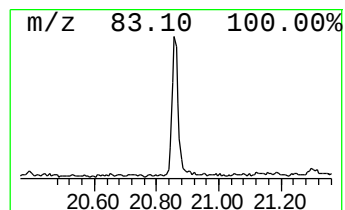
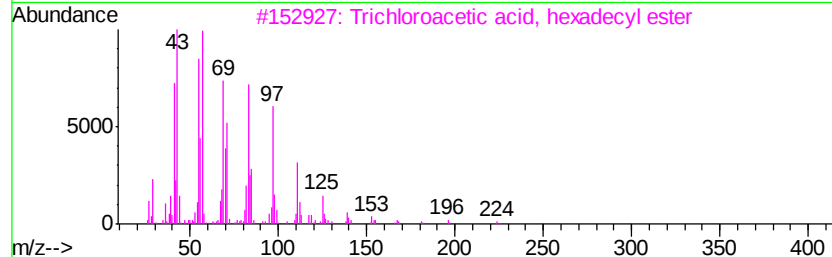
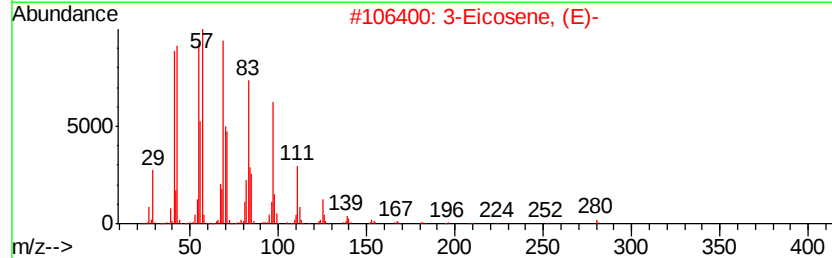
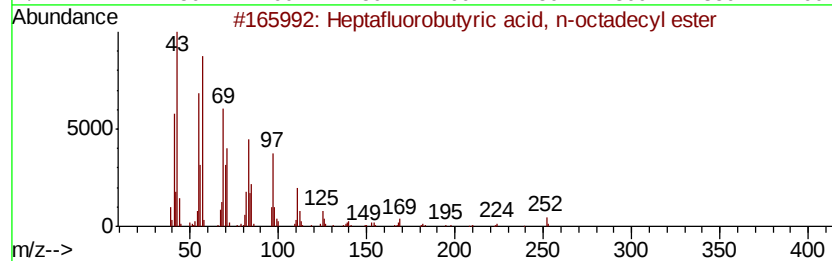
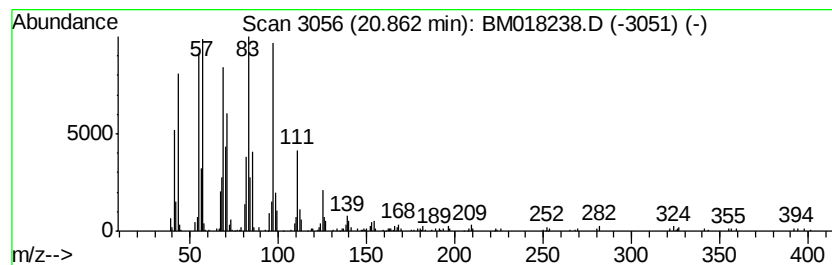
Instrument :
BNA_M
ClientSampleId :
P001-SS005-1824-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.86	8.42 ng	629971	Chrysene-d12		21.14	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		Trichloroacetic acid, hexadecyl ester	386	C18H33Cl3O2	074339-54-1	91
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121618\
Data File : BM018238.D
Acq On : 16 Dec 2018 22:12
Operator : JU/SJ
Sample : J6386-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SS005-1824-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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
Propylene Glycol	3.36	2.8	ng	121053	1	7.50	856621	20.0
2-Pentanone, 4-hy...	4.69	3.4	ng	147524	1	7.50	856621	20.0
unknown7.04	7.04	116.1	ng	4971630	1	7.50	856621	20.0
n-Hexadecanoic acid	17.83	7.0	ng	522224	4	16.92	1493940	20.0
Octadecanoic acid	19.13	2.2	ng	163763	5	21.14	1496360	20.0
Heptafluorobutyri...	20.86	8.4	ng	629971	5	21.14	1496360	20.0