

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016291.D
Acq On : 09 Aug 2018 20:56
Operator : SJ/JU
Sample : J4380-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-08

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	332	rBV	36466	56276	2.08%	0.429%
2	5.663	399	404	414	rBV	321629	518854	19.19%	3.956%
3	7.310	678	684	695	rBV	171410	303704	11.23%	2.316%
4	7.663	737	744	762	rBV	762583	1239458	45.85%	9.451%
5	8.128	818	823	833	rBV	165746	271298	10.04%	2.069%
6	8.451	871	878	890	rBB	752277	1197531	44.30%	9.131%
7	9.316	1019	1025	1037	rBV	552704	935921	34.62%	7.136%
8	10.945	1295	1302	1312	rBV	174550	304064	11.25%	2.319%
9	13.386	1709	1717	1726	rBV	1279309	1798841	66.54%	13.716%
10	14.221	1853	1859	1871	rVB	78052	115774	4.28%	0.883%
11	14.763	1945	1951	1958	rBV2	217057	339194	12.55%	2.586%
12	15.745	2110	2118	2122	rBV	27111	40328	1.49%	0.308%
13	16.257	2199	2205	2217	rVB	1062902	1497270	55.38%	11.417%
14	16.621	2262	2267	2273	rVB4	17966	34078	1.26%	0.260%
15	16.880	2307	2311	2318	rVB6	18497	32776	1.21%	0.250%
16	17.504	2411	2417	2423	rBV2	260922	374494	13.85%	2.856%
17	18.351	2557	2561	2572	rBV	135158	200413	7.41%	1.528%
18	18.927	2656	2659	2664	rVB7	23384	31174	1.15%	0.238%
19	19.609	2772	2775	2779	rBV2	49732	68697	2.54%	0.524%
20	20.080	2849	2855	2862	rBV	2283380	2703407	100.00%	20.614%
21	21.297	3059	3062	3067	rBV3	65892	84166	3.11%	0.642%
22	21.633	3114	3119	3125	rBV	368889	489461	18.11%	3.732%
23	23.968	3511	3516	3523	rVB	247296	477479	17.66%	3.641%

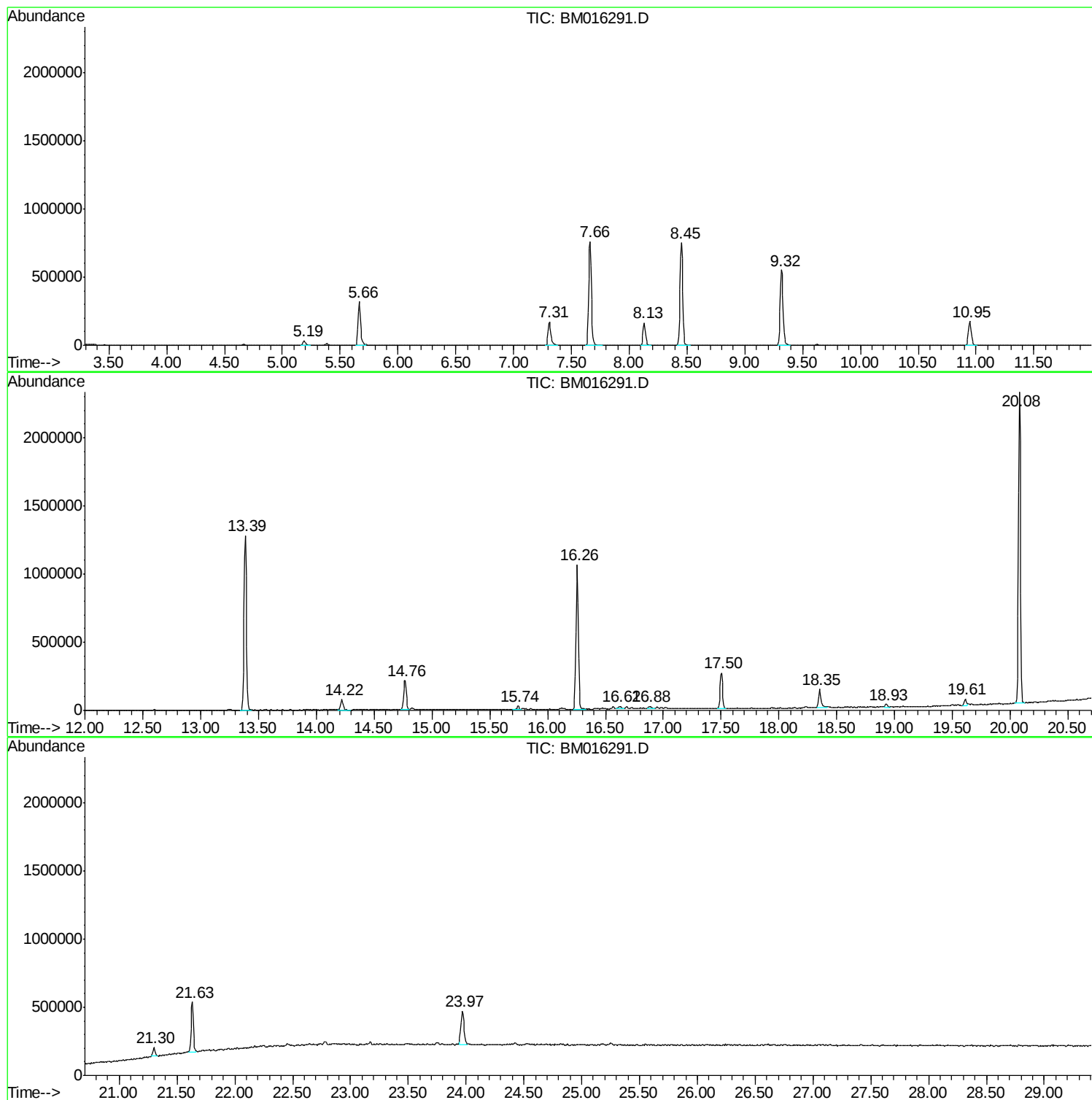
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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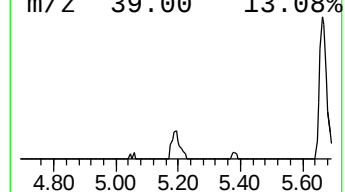
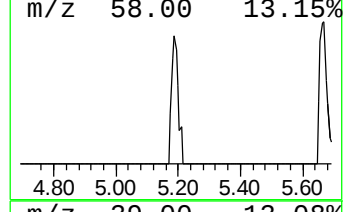
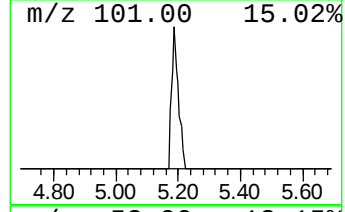
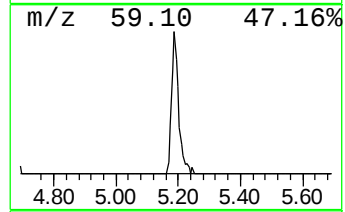
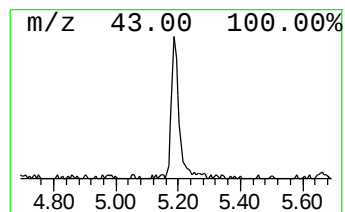
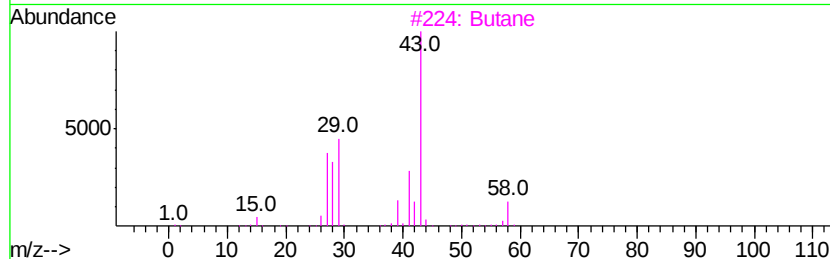
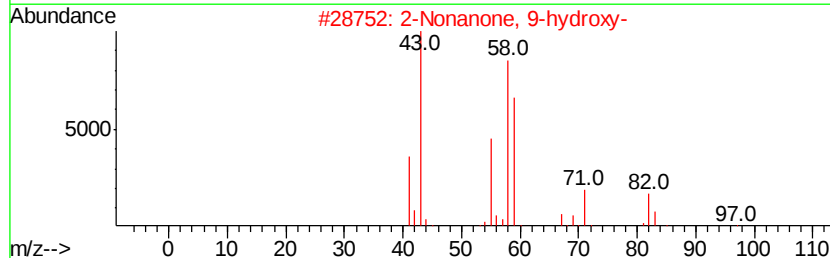
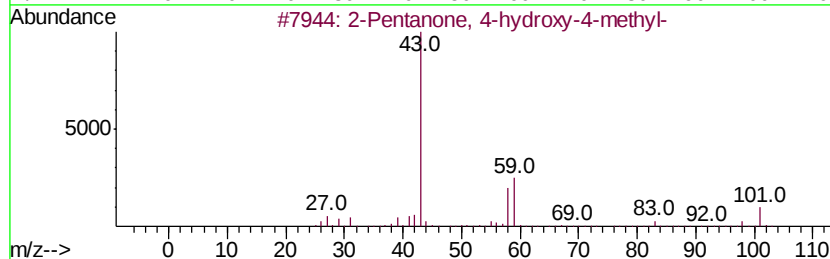
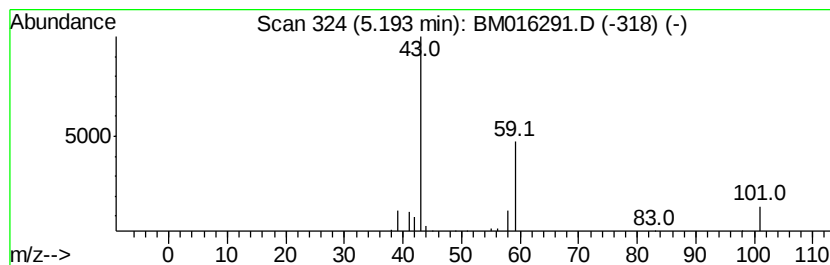
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	4.15 ng	56276	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	38
3	Butane	58	C4H10	000106-97-8	16
4	Propylamine	59	C3H9N	000107-10-8	9
5	2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	9



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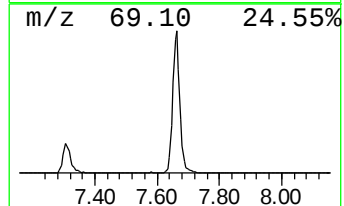
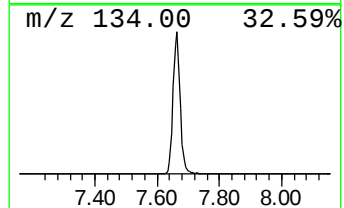
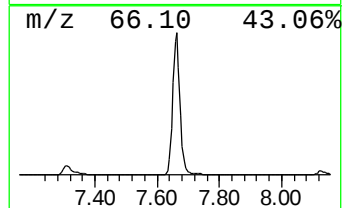
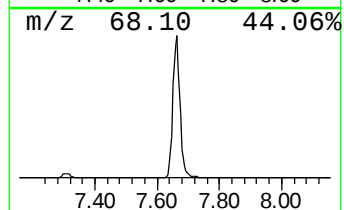
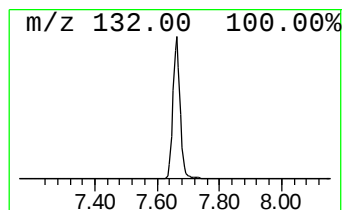
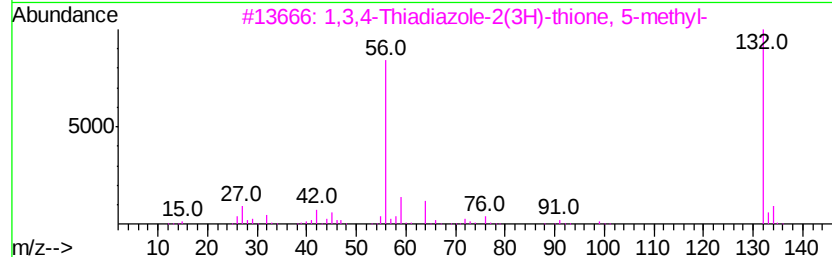
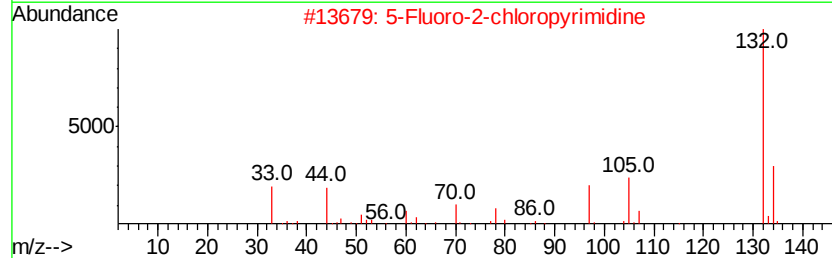
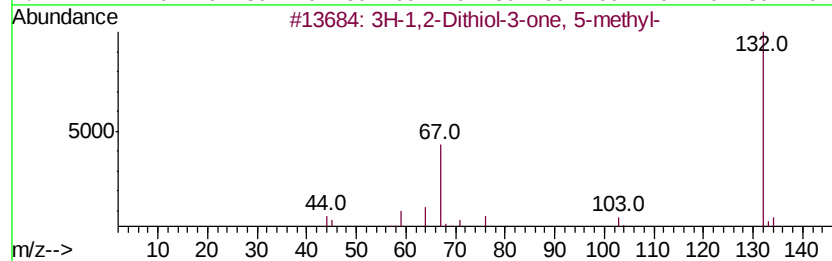
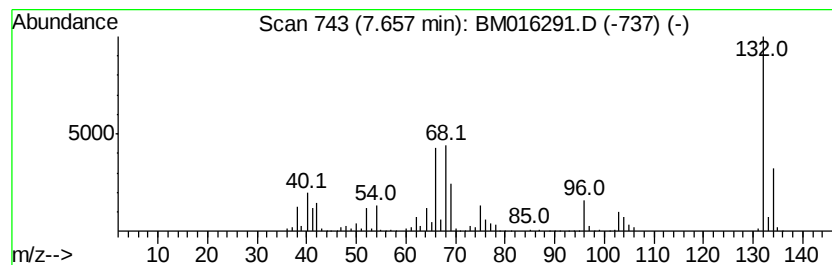
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Peak Number 2 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	91.37 ng	1239460	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	14



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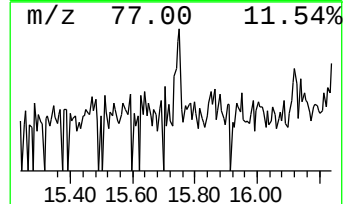
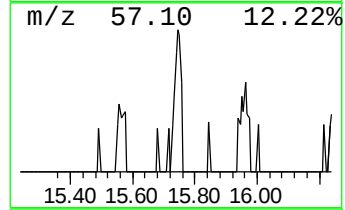
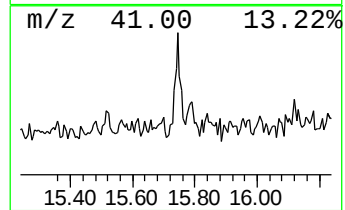
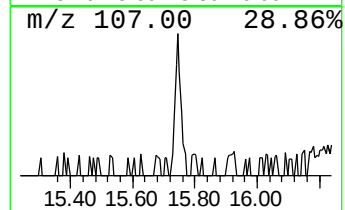
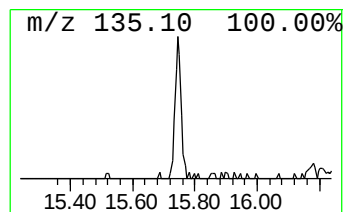
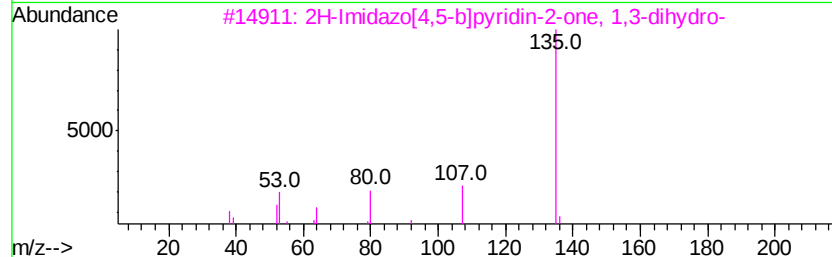
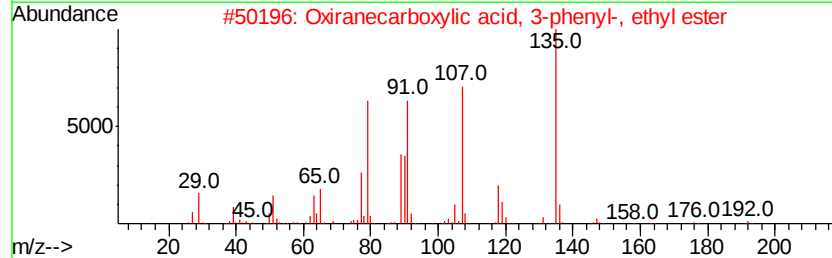
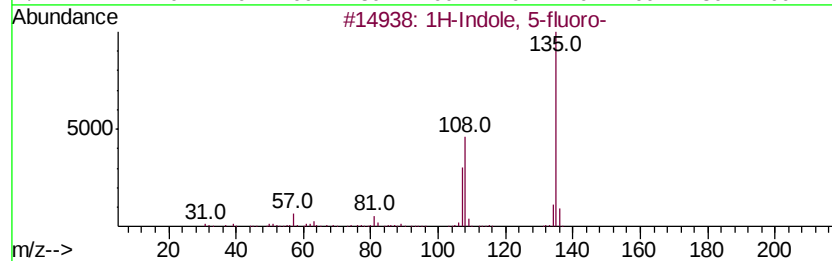
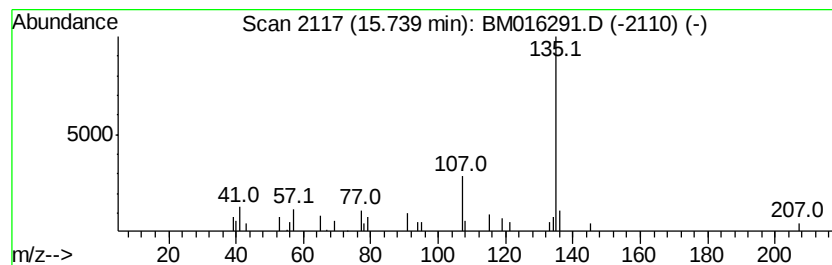
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Peak Number 4 1H-Indole, 5-fluoro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.38 ng	40328	Acenaphthene-d10	14.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	72
2		Oxiranecarboxylic acid, 3-phenyl...	192	C11H12O3	000121-39-1	59
3		2H-Imidazo[4,5-b]pyridin-2-one, ...	135	C6H5N3O	016328-62-4	59
4		Phenol, 4,4'-(1,2-diethyl-1,2-et...	270	C18H22O2	000084-16-2	50
5		1-Cyclopentenecarboxylic acid, 2...	246	C15H15FO2	1000158-81-1	45



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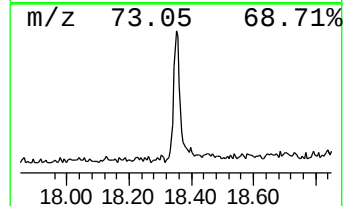
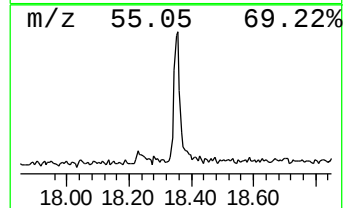
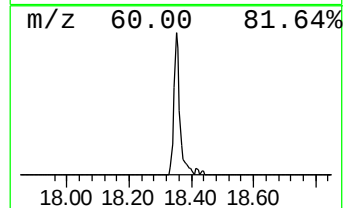
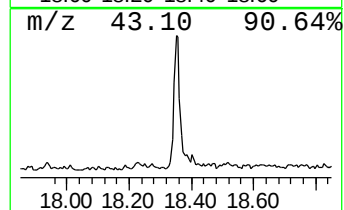
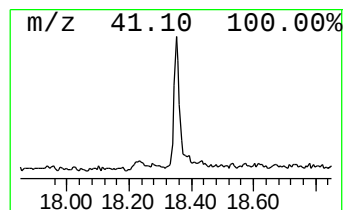
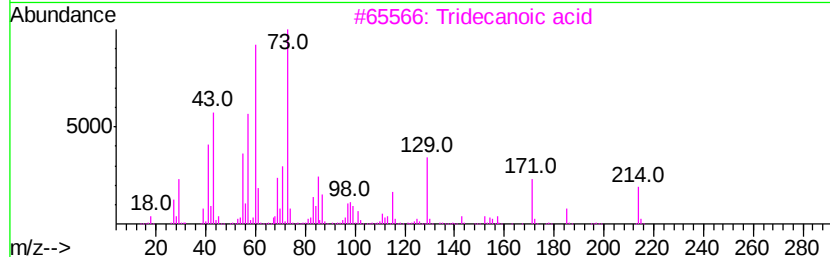
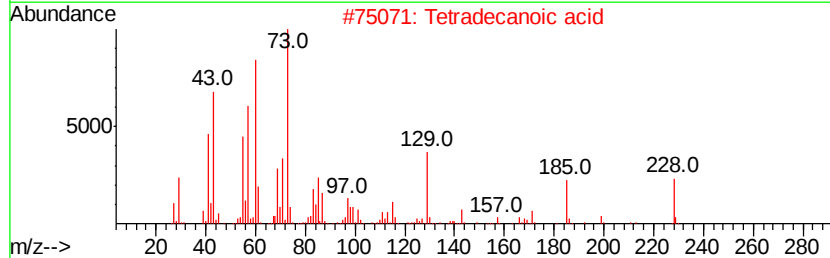
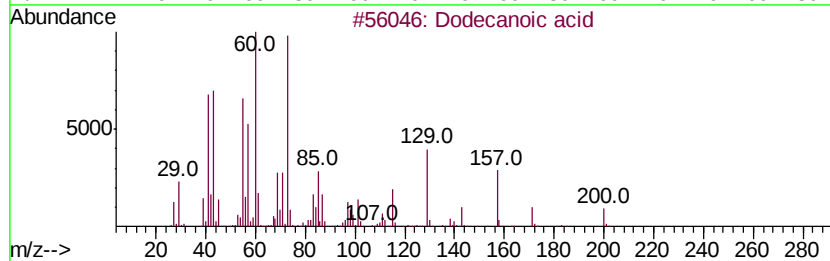
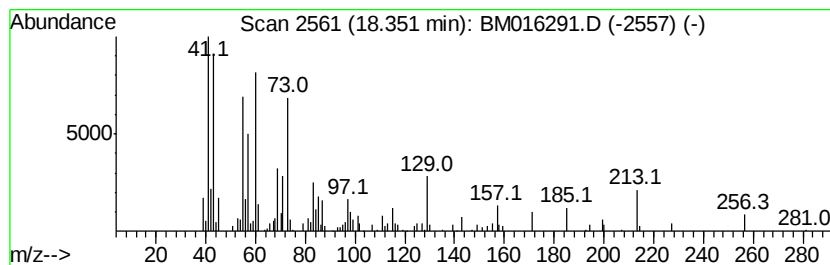
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Peak Number 5 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	10.70 ng	200413	Phenanthrene-d10	17.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecanoic acid	200	C12H24O2	000143-07-7	64
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3		Tridecanoic acid	214	C13H26O2	000638-53-9	59
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
5		Nonanoic acid	158	C9H18O2	000112-05-0	53



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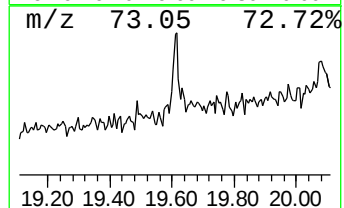
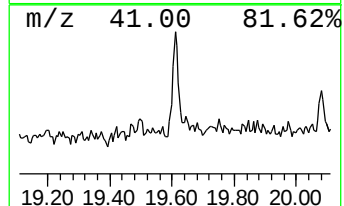
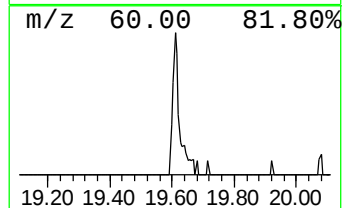
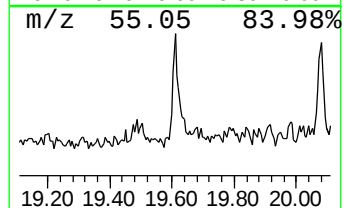
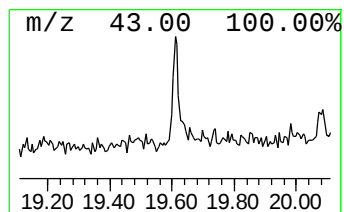
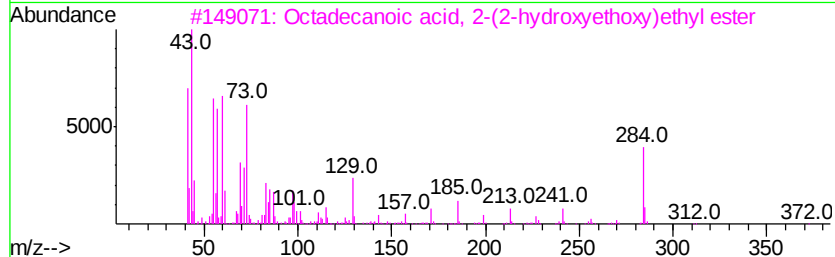
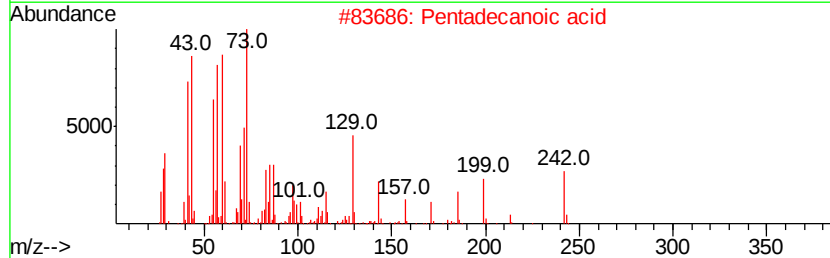
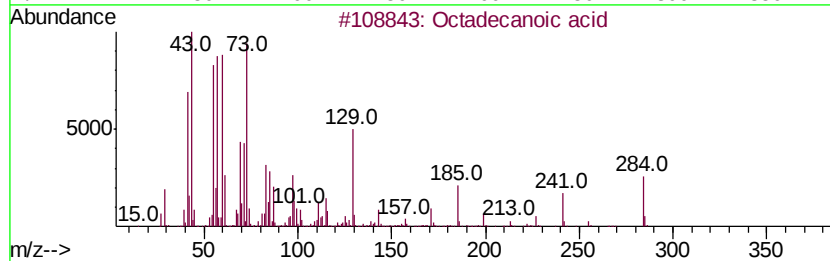
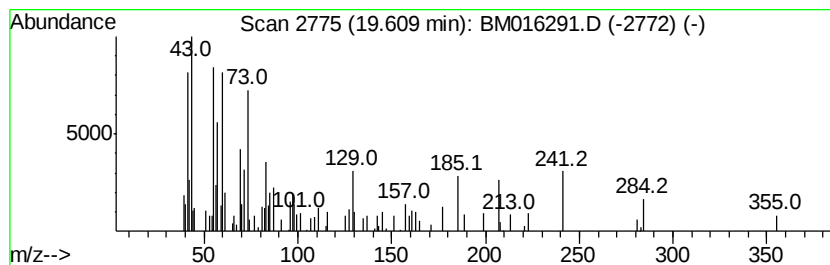
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Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	2.81 ng	68697	Chrysene-d12	21.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	68
3	Octadecanoic acid, 2-(2-hydroxyve...		372	C22H44O4	000106-11-6	59
4	Tridecanoic acid		214	C13H26O2	000638-53-9	47
5	Undecanoic acid		186	C11H22O2	000112-37-8	47



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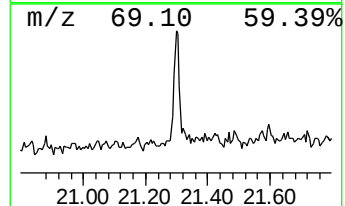
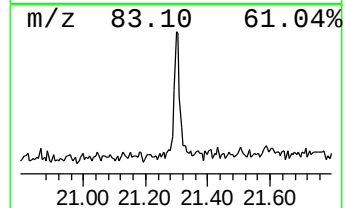
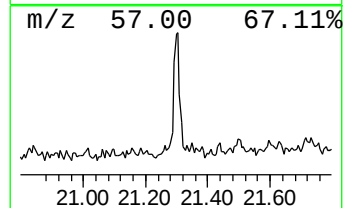
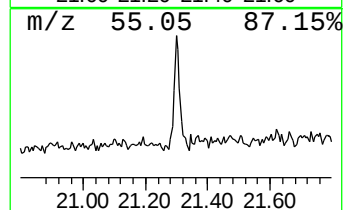
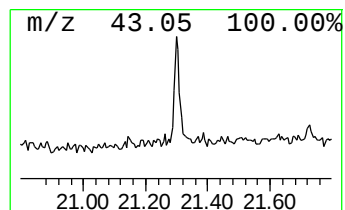
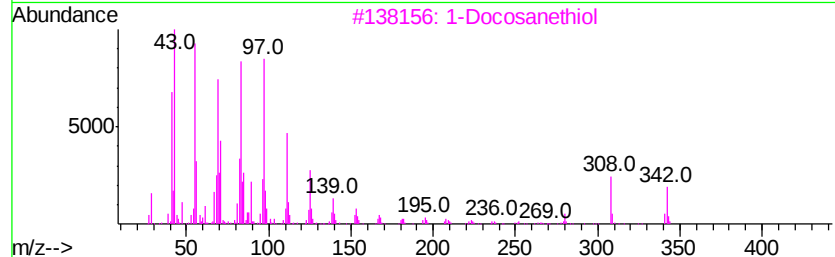
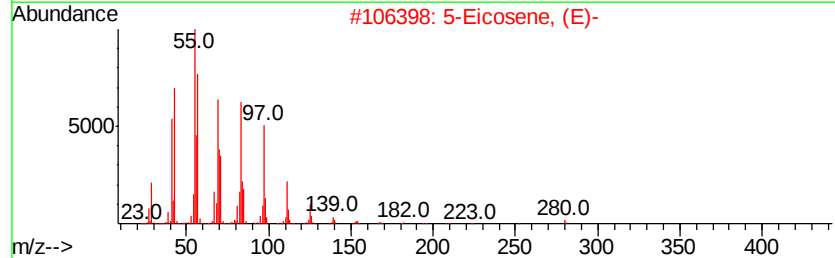
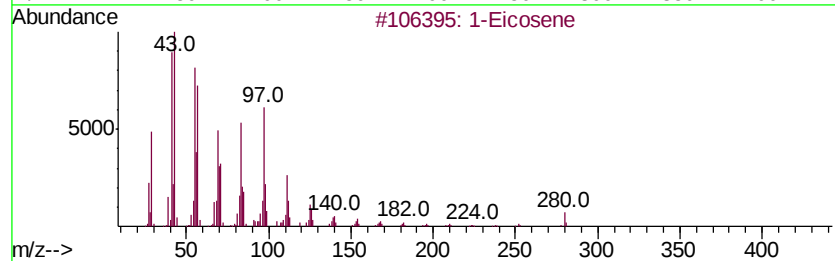
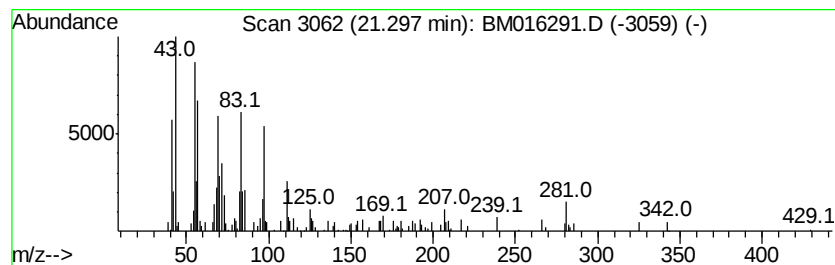
Instrument :
BNA_M
ClientSampleId :
MW-08

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 1-Eicosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.30	3.44 ng	84166	Chrysene-d12	21.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	1-Docosanethiol	342	C22H46S	007773-83-3	87
4	4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	83
5	Cycloeicosane	280	C20H40	000296-56-0	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080918\
Data File : BM016291.D
Acq On : 09 Aug 2018 20:56
Operator : SJ/JU
Sample : J4380-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-08

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...	5.19	4.2	ng	56276	1	8.13	271298	20.0
unknown7.66	7.66	91.4	ng	1239460	1	8.13	271298	20.0
1H-Indole, 5-fluoro-	15.74	2.4	ng	40328	3	14.76	339194	20.0
Dodecanoic acid	18.35	10.7	ng	200413	4	17.50	374494	20.0
Octadecanoic acid	19.61	2.8	ng	68697	5	21.63	489461	20.0
1-Eicosene	21.30	3.4	ng	84166	5	21.63	489461	20.0