

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
 Data File : BF101971.D
 Acq On : 9 Jan 2018 23:45
 Operator : SJ/JU
 Sample : J1049-10
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-E

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:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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	4.922	478	482	488	rVB	181879	220934	3.85%	0.551%
2	5.334	547	552	555	rBV	2907332	2811296	48.94%	7.015%
3	6.357	721	726	734	rVB	1976482	1735746	30.22%	4.331%
4	6.498	745	750	753	rBV	5011592	4974065	86.59%	12.411%
5	6.728	785	789	792	rBV	1801780	1414555	24.62%	3.530%
6	6.793	797	800	804	rVB2	90131	73786	1.28%	0.184%
7	6.887	811	816	819	rBV	5193321	4964146	86.42%	12.386%
8	6.910	819	820	823	rVB2	112274	60469	1.05%	0.151%
9	7.298	878	886	889	rBV	3960151	4170578	72.60%	10.406%
10	7.487	915	918	921	rVB	76047	59698	1.04%	0.149%
11	7.898	983	988	990	rBV2	52296	60706	1.06%	0.151%
12	8.010	1001	1007	1010	rBV	2210155	1769836	30.81%	4.416%
13	8.257	1047	1049	1055	rVB7	41101	58808	1.02%	0.147%
14	8.375	1065	1069	1072	rBV3	55695	74962	1.30%	0.187%
15	8.569	1099	1102	1106	rBV	103228	100684	1.75%	0.251%
16	8.986	1170	1173	1179	rBV8	36554	72330	1.26%	0.180%
17	9.092	1185	1191	1194	rBV	6050486	5744409	100.00%	14.333%
18	9.186	1203	1207	1209	rBV4	55451	74788	1.30%	0.187%
19	9.481	1255	1257	1259	rVB2	81091	60950	1.06%	0.152%
20	9.686	1288	1292	1296	rVB	404384	412502	7.18%	1.029%
21	9.763	1302	1305	1308	rVV	1665757	1354910	23.59%	3.381%
22	9.792	1308	1310	1314	rVB2	88891	77038	1.34%	0.192%
23	10.316	1396	1399	1401	rVB2	104990	93113	1.62%	0.232%
24	10.480	1425	1427	1430	rBV	126491	95962	1.67%	0.239%
25	10.551	1435	1439	1442	rBV	2528716	2456167	42.76%	6.129%
26	11.245	1554	1557	1563	rVB	1342702	1185091	20.63%	2.957%
27	11.792	1647	1650	1655	rBV2	282737	270513	4.71%	0.675%
28	11.969	1677	1680	1684	rVB	209946	186854	3.25%	0.466%
29	12.574	1781	1783	1787	rBV	291610	279710	4.87%	0.698%
30	12.839	1824	1828	1831	rBV	3532864	3290869	57.29%	8.211%
31	13.886	2002	2006	2009	rBV	1241011	1090475	18.98%	2.721%
32	15.304	2243	2247	2253	rVB	639217	781200	13.60%	1.949%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

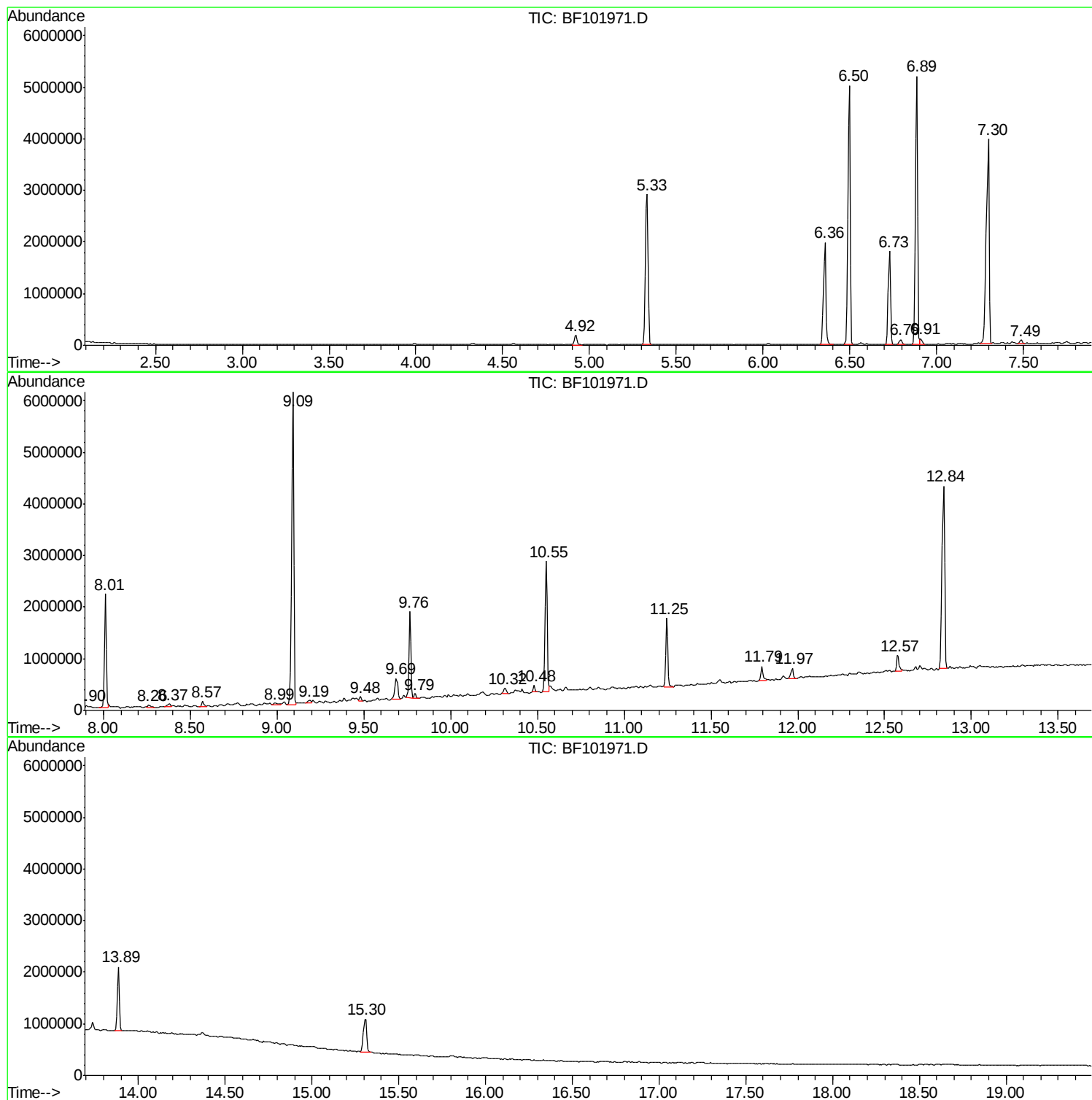
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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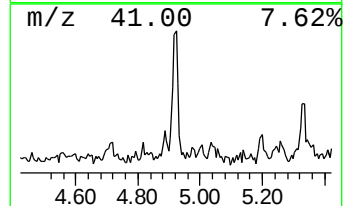
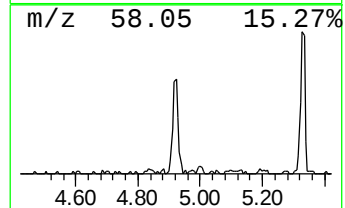
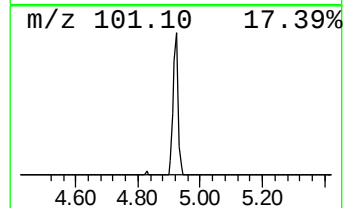
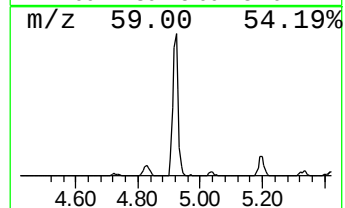
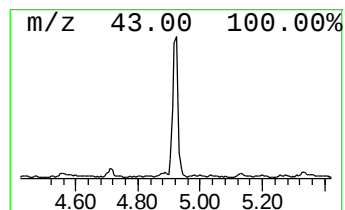
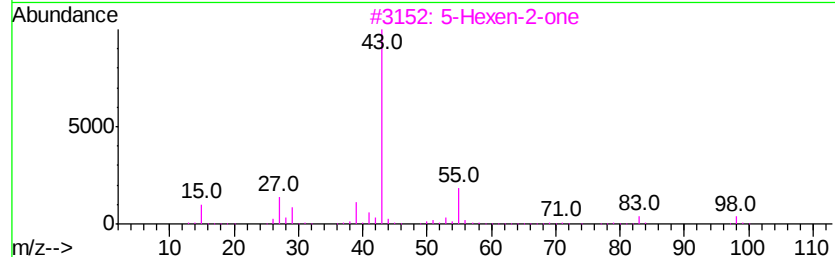
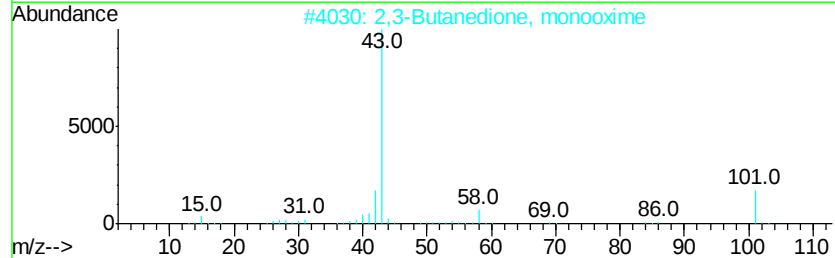
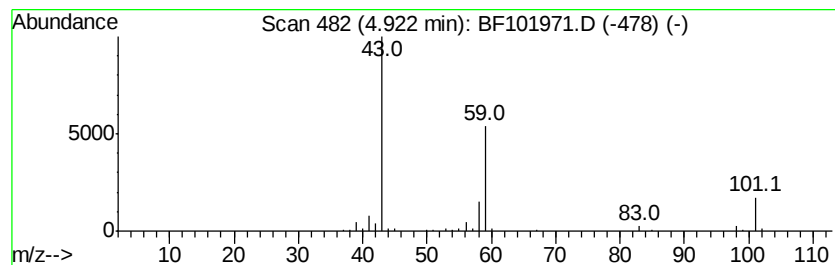
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.12 ng	220934	1,4-Dichlorobenzene-d4	6.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9	



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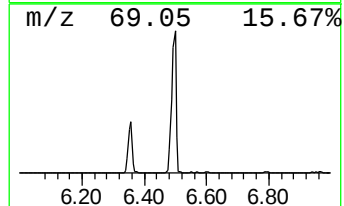
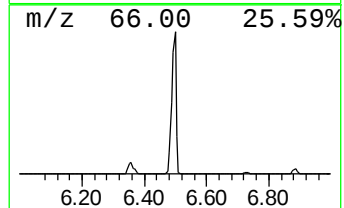
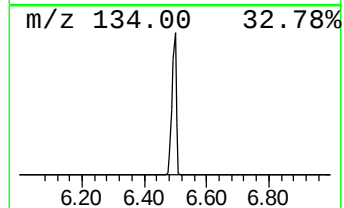
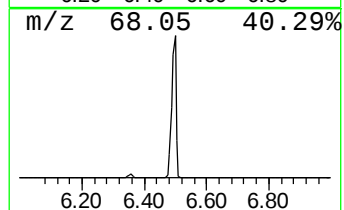
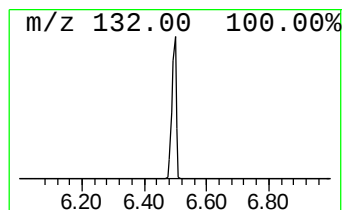
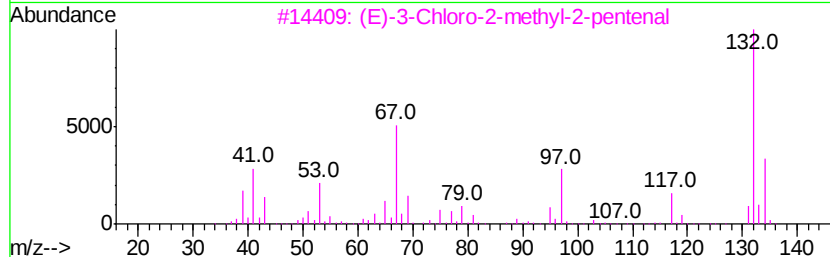
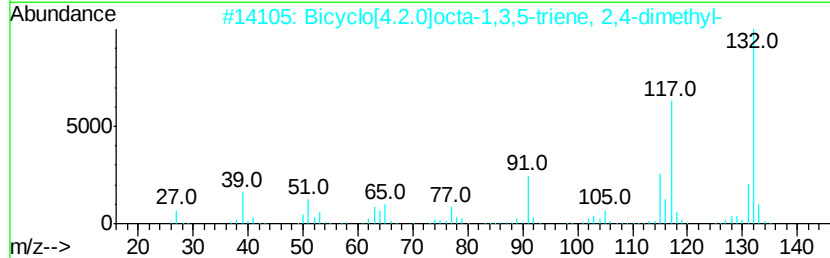
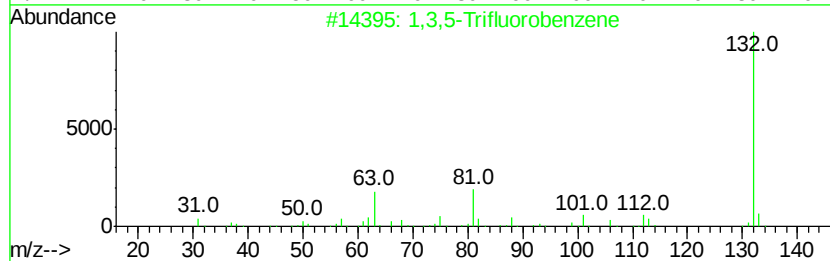
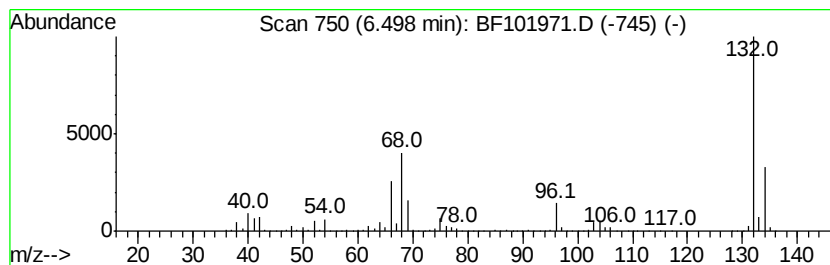
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	70.33 ng	4974070	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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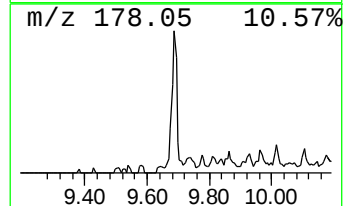
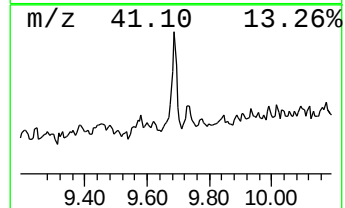
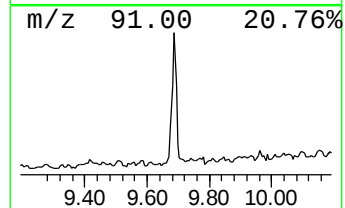
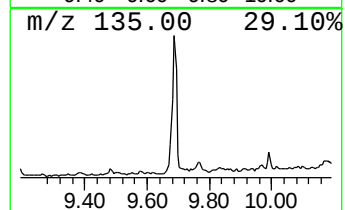
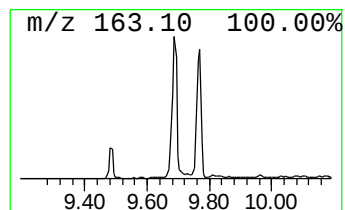
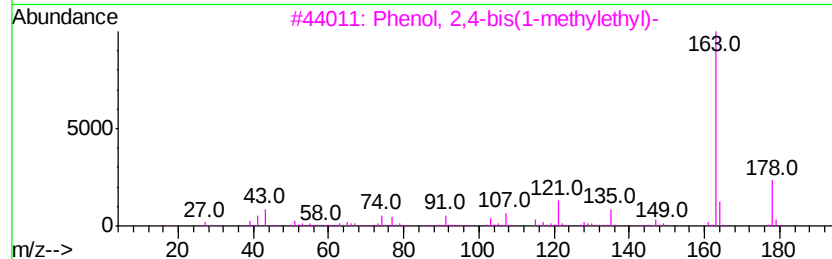
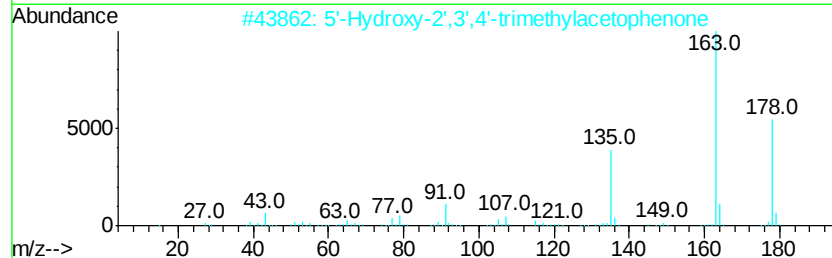
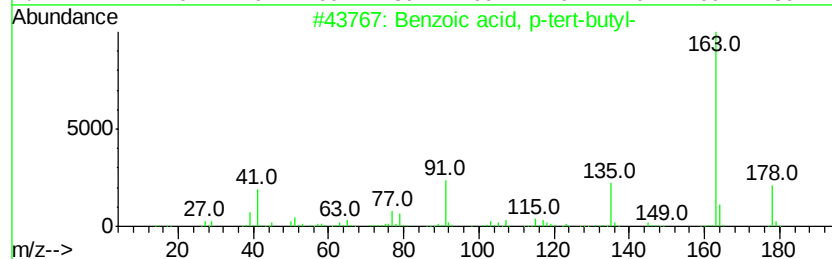
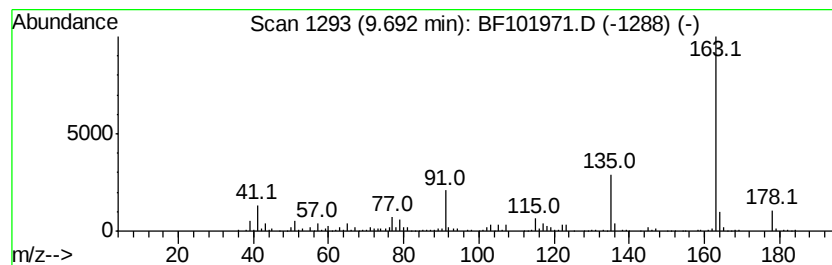
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzoic acid, p-tert-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	6.09 ng	412502	Acenaphthene-d10	9.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	95
2		5'-Hydroxy-2',3',4'-trimethylace...	178	C11H14O2	013667-28-2	64
3		Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	59
4		1,4-Cyclohexadiene, 3,3,6,6-tetr...	192	C14H24	078578-89-9	59
5		Silane, (4-ethylphenyl)trimethyl-	178	C11H18Si	017988-50-0	58



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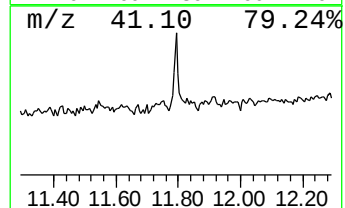
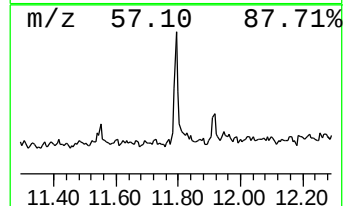
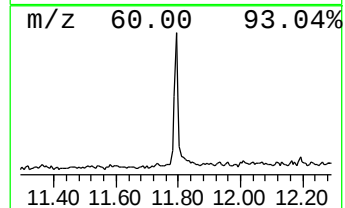
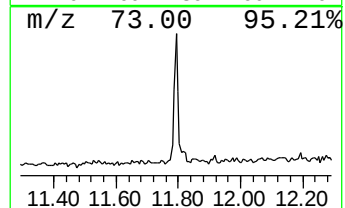
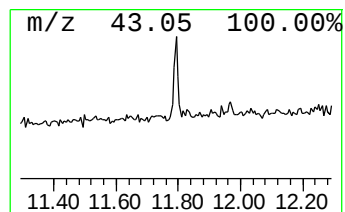
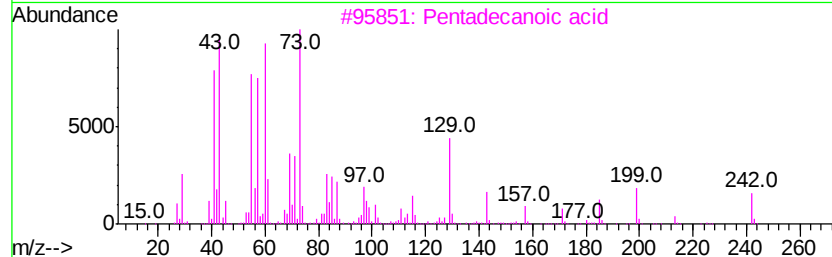
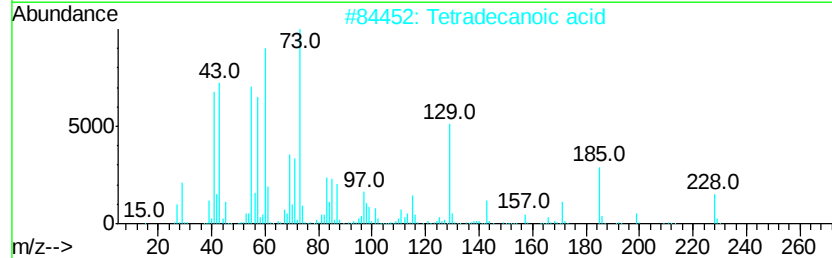
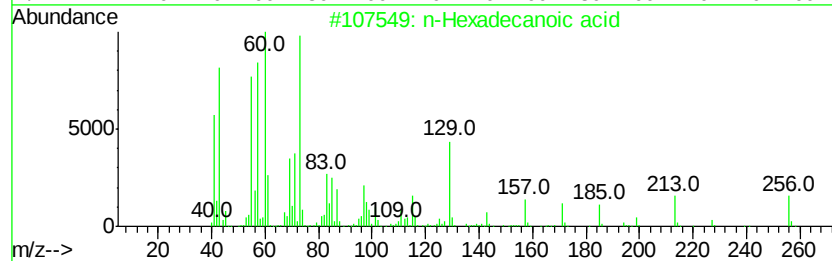
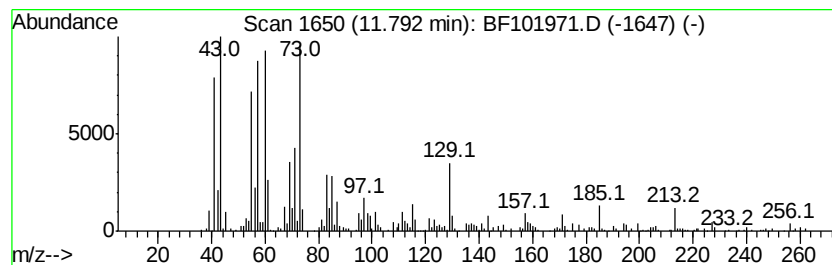
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	4.57 ng	270513	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Undecanoic acid	186	C11H22O2	000112-37-8	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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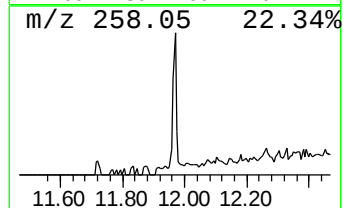
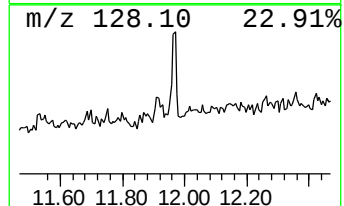
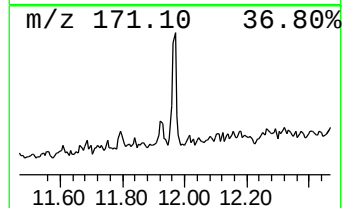
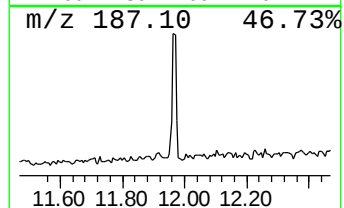
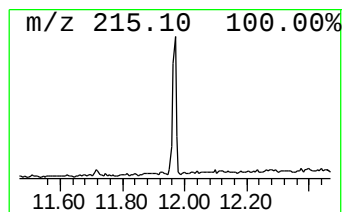
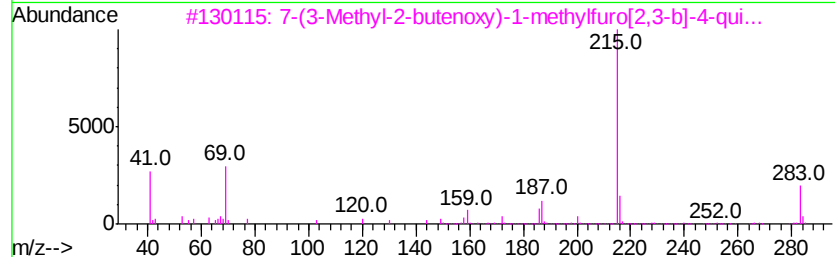
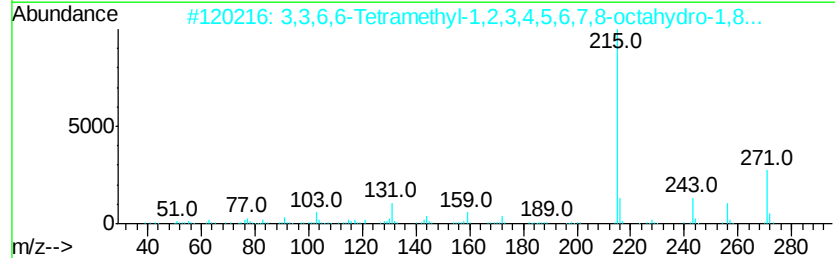
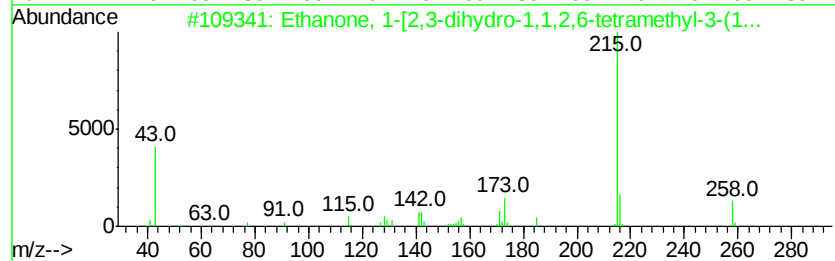
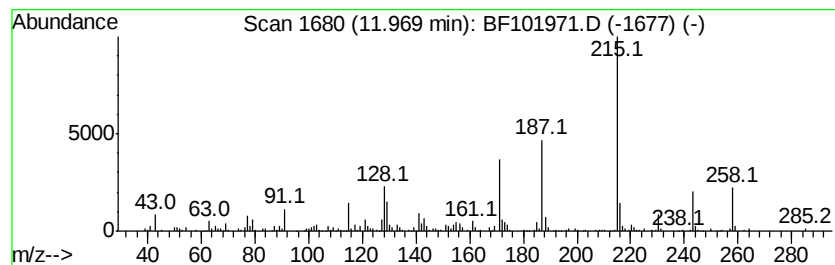
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Peak Number 6 unknown11.97 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	3.15 ng	186854	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-[2,3-dihydro-1,1,2,6...	258	C18H26O	068140-48-7	37
2		3,3,6,6-Tetramethyl-1,2,3,4,5,6,...	271	C17H21NO2	027361-25-7	35
3		7-(3-Methyl-2-butenoxv)-1-methyl...	283	C17H17NO3	1000100-62-4	35
4		2-Thiophen-2-yl-imidazo[1,2-a]py...	215	C11H9N3S	1000300-55-5	35
5		2,3-Methanonaphthalene-9-carboxa...	215	C14H17NO	030265-04-4	32



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MW-E

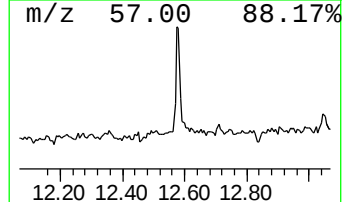
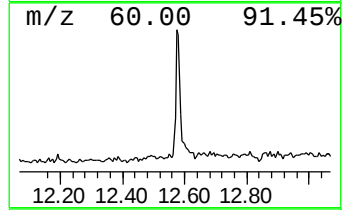
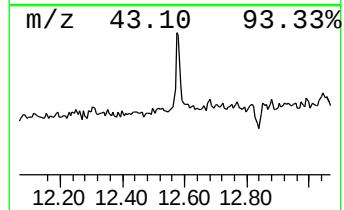
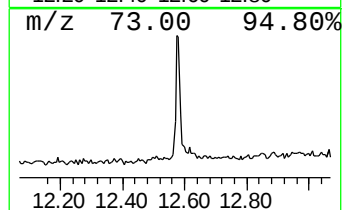
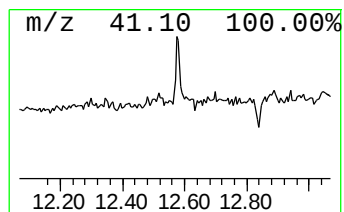
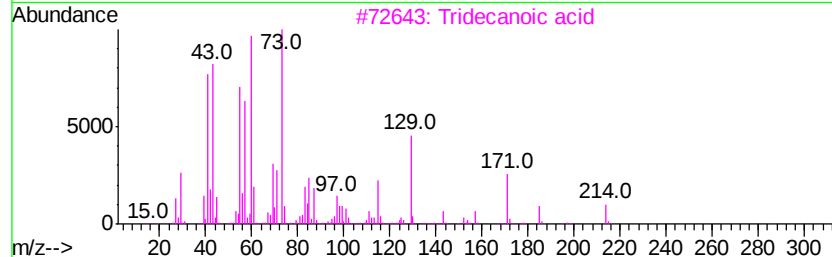
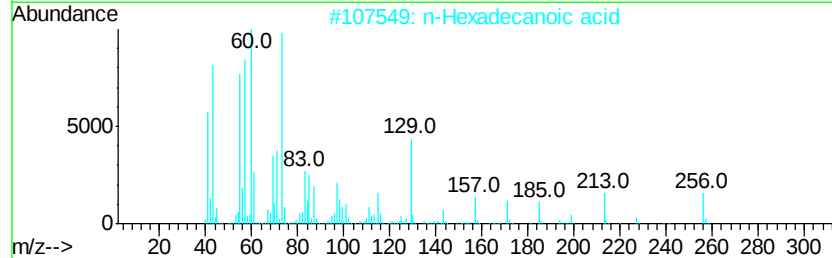
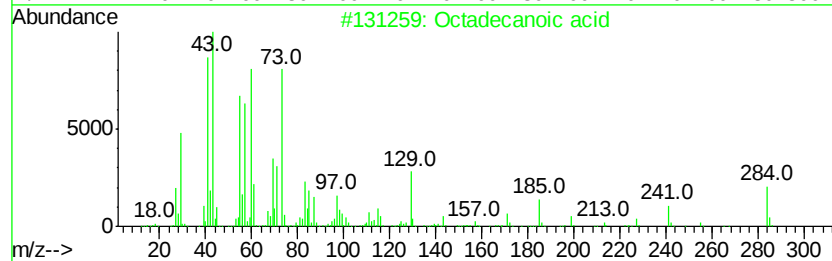
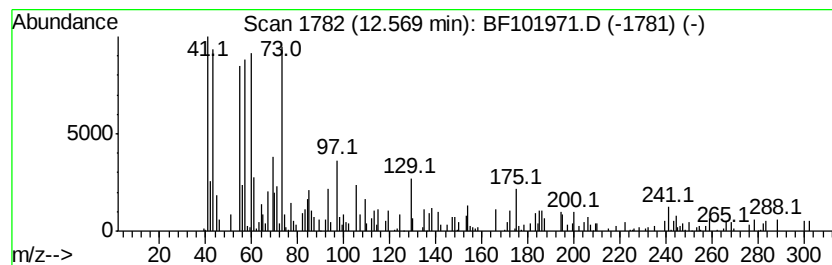
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	5.13 ng	279710	Chrysene-d12	13.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	60
5			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	60



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
Data File : BF101971.D
Acq On : 9 Jan 2018 23:45
Operator : SJ/JU
Sample : J1049-10
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	3.1	ng	220934	1	6.73	1414560	20.0
unknown6.50	6.50	70.3	ng	4974070	1	6.73	1414560	20.0
Benzoic acid, p-t...	9.69	6.1	ng	412502	3	9.76	1354910	20.0
n-Hexadecanoic acid	11.79	4.6	ng	270513	4	11.25	1185090	20.0
unknown11.97	11.97	3.1	ng	186854	4	11.25	1185090	20.0
Octadecanoic acid	12.57	5.1	ng	279710	5	13.89	1090480	20.0