

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
 Data File : BF101606.D
 Acq On : 21 Dec 2017 14:56
 Operator : SJ/JU
 Sample : I6966-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DB-WATER

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-BF121417.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	5.004	493	496	514	rVB	102700	174360	5.36%	0.723%
2	5.416	563	566	590	rBV	1157742	1583612	48.65%	6.571%
3	6.439	737	740	758	rBV	733299	1118147	34.35%	4.639%
4	6.569	758	762	773	rVV	2722927	2603551	79.99%	10.802%
5	6.798	797	801	807	rBV	791407	786564	24.17%	3.264%
6	6.851	807	810	817	rVB2	32007	48444	1.49%	0.201%
7	6.951	823	827	843	rBV	2672343	2518480	77.37%	10.449%
8	7.369	893	898	913	rBV	1903577	2105999	64.70%	8.738%
9	7.816	968	974	977	rBV3	62788	63334	1.95%	0.263%
10	8.075	1015	1018	1033	rVB	971788	985587	30.28%	4.089%
11	8.269	1047	1051	1058	rBV8	17907	34974	1.07%	0.145%
12	8.439	1077	1080	1086	rBV4	27619	45034	1.38%	0.187%
13	9.016	1175	1178	1183	rBV	53410	52293	1.61%	0.217%
14	9.151	1195	1201	1204	rBV	3422648	3254909	100.00%	13.505%
15	9.257	1215	1219	1223	rBV	175817	171391	5.27%	0.711%
16	9.545	1265	1268	1271	rBV	76678	68226	2.10%	0.283%
17	9.575	1271	1273	1277	rVB	56626	46938	1.44%	0.195%
18	9.798	1308	1311	1313	rBV	54200	55807	1.71%	0.232%
19	9.833	1313	1317	1321	rVV	986558	880347	27.05%	3.653%
20	10.022	1346	1349	1352	rBV	124463	121988	3.75%	0.506%
21	10.063	1354	1356	1359	rVB	47013	44929	1.38%	0.186%
22	10.163	1371	1373	1380	rVB2	36494	33482	1.03%	0.139%
23	10.222	1380	1383	1386	rBV	531481	437986	13.46%	1.817%
24	10.245	1386	1387	1391	rVB	49437	40011	1.23%	0.166%
25	10.627	1448	1452	1460	rBV	1606582	1587511	48.77%	6.587%
26	10.751	1471	1473	1479	rVB3	28021	34853	1.07%	0.145%
27	10.869	1490	1493	1498	rVB	58134	57387	1.76%	0.238%
28	10.980	1510	1512	1522	rBV6	38684	63000	1.94%	0.261%
29	11.080	1527	1529	1534	rVB	44852	45441	1.40%	0.189%
30	11.286	1561	1564	1567	rBV	36652	33848	1.04%	0.140%
31	11.322	1567	1570	1578	rVB	818720	787793	24.20%	3.269%
32	11.692	1631	1633	1638	rVB3	52835	52165	1.60%	0.216%
33	11.839	1655	1658	1663	rBV	85227	99760	3.06%	0.414%
34	12.621	1789	1791	1796	rBV5	60521	91047	2.80%	0.378%

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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

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35	12.674	1798	1800	1802	rBV2	42429	39895	1.23%	0.166%
36	12.910	1835	1840	1843	rBV	2545704	2520025	77.42%	10.456%
37	13.974	2017	2021	2024	rBV	833640	783741	24.08%	3.252%
38	15.439	2266	2270	2275	rVB	538932	628775	19.32%	2.609%

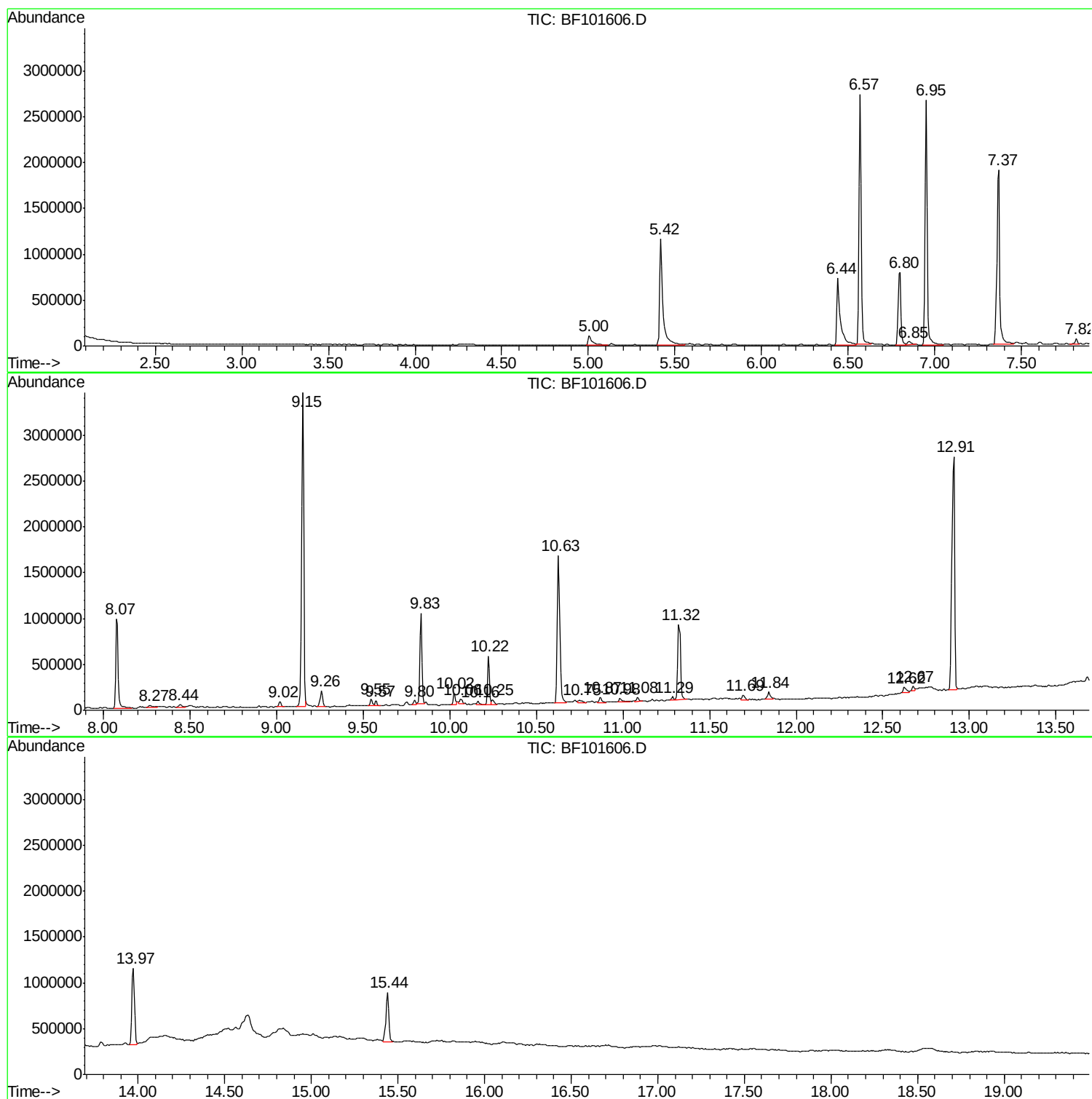
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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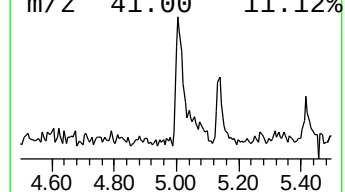
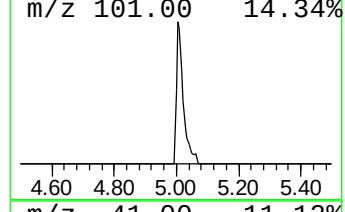
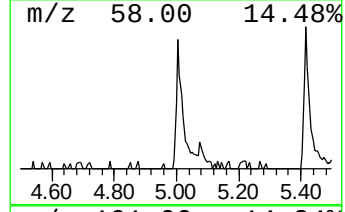
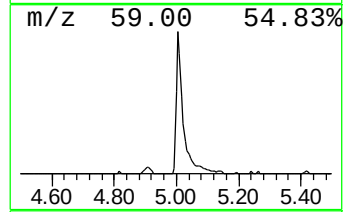
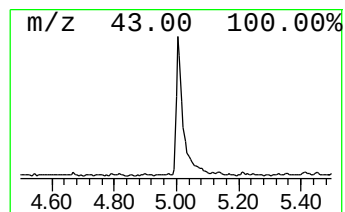
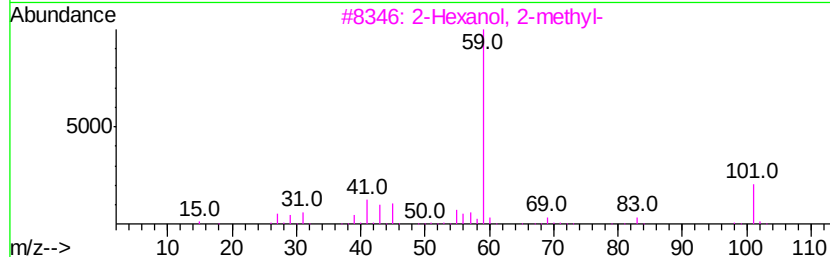
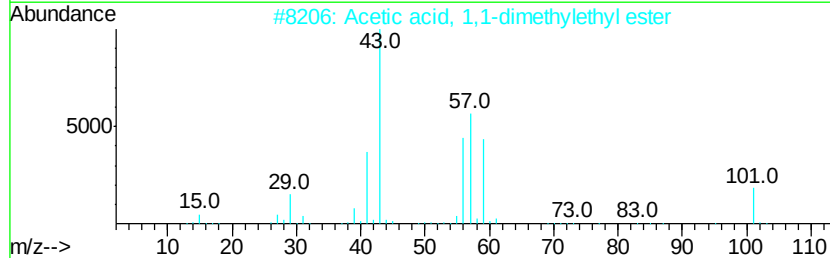
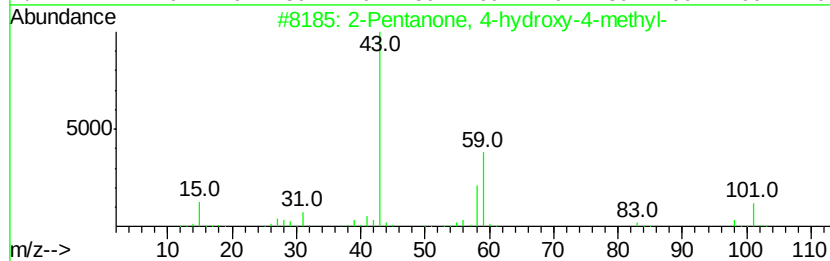
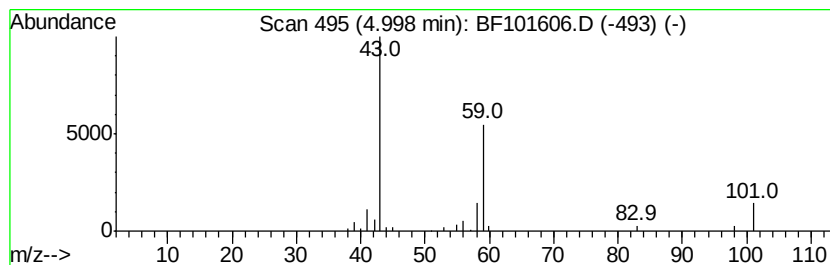
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.00	4.43 ng	174360	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23



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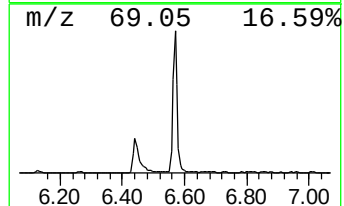
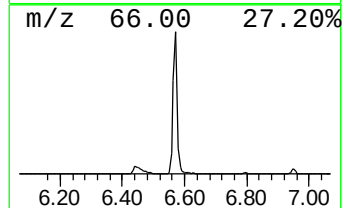
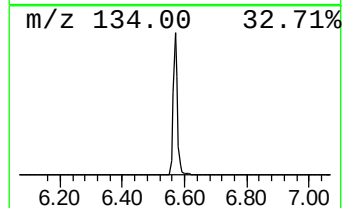
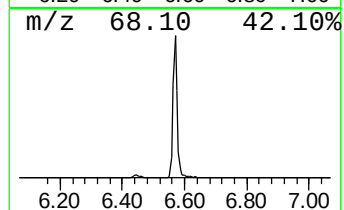
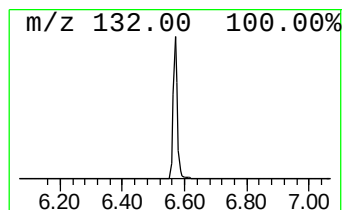
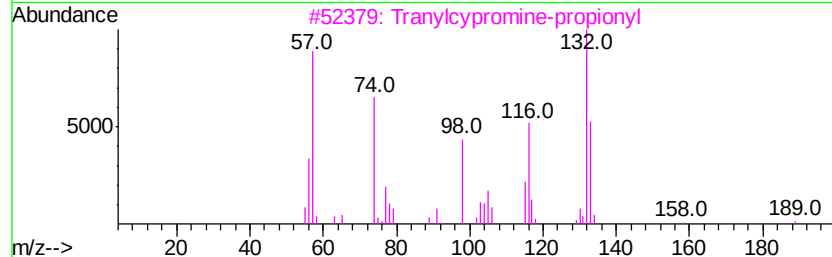
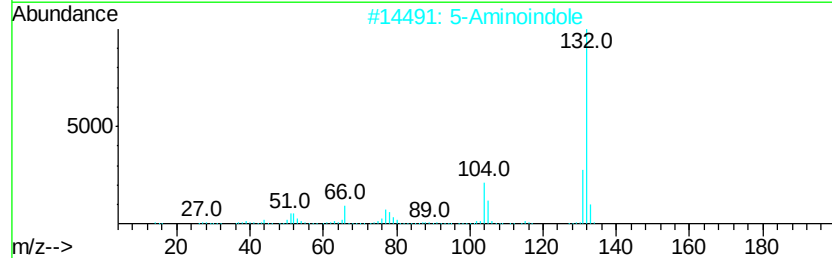
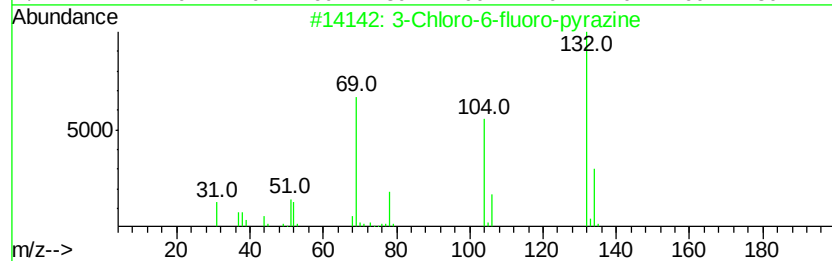
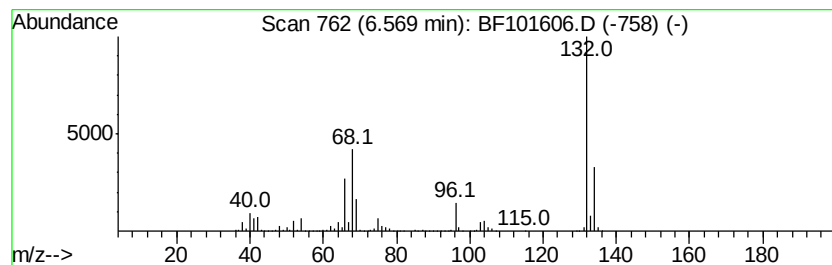
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	66.20 ng	2603550	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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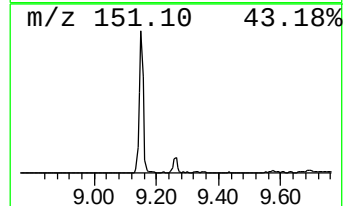
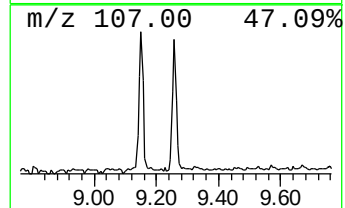
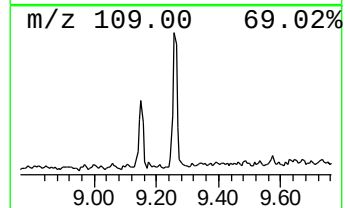
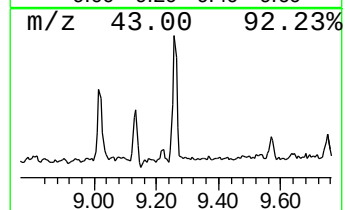
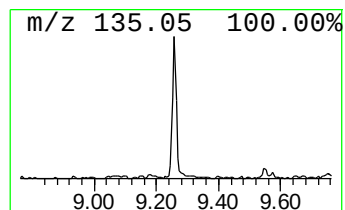
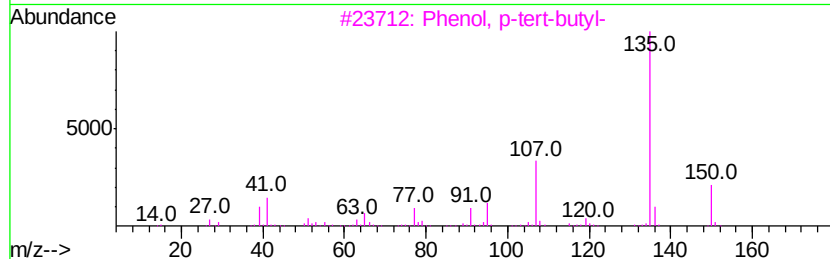
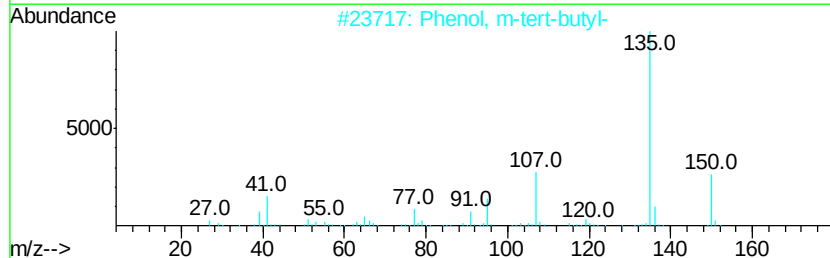
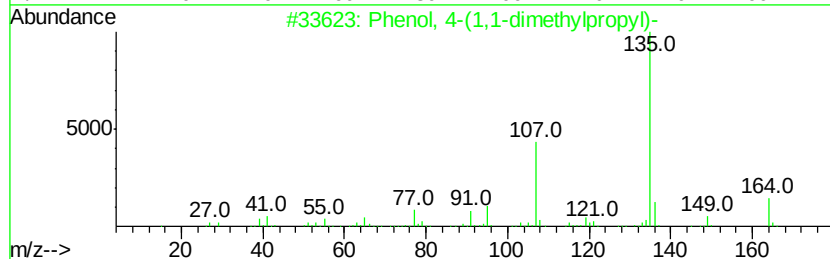
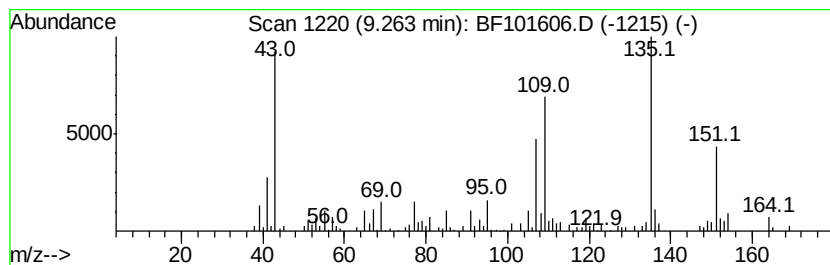
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenol, 4-(1,1-dimethylprop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.26	3.89 ng	171391	Acenaphthene-d10	9.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	91		
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	53		
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	47		
4	p-Methoxybenzamide	151	C8H9NO2	003424-93-9	43		
5	Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	000501-00-8	43		



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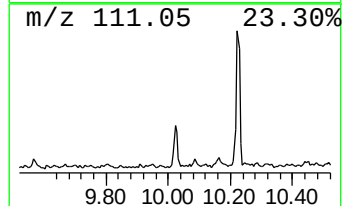
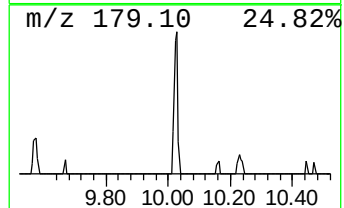
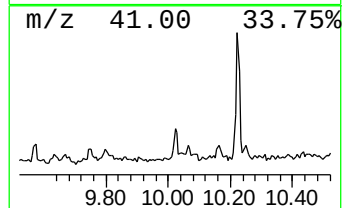
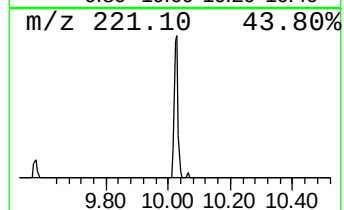
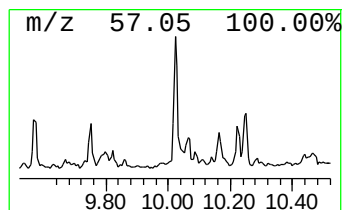
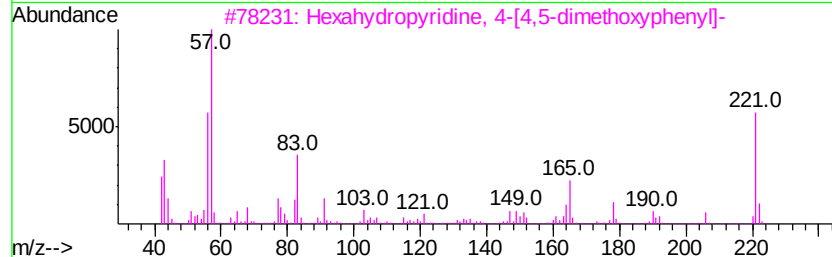
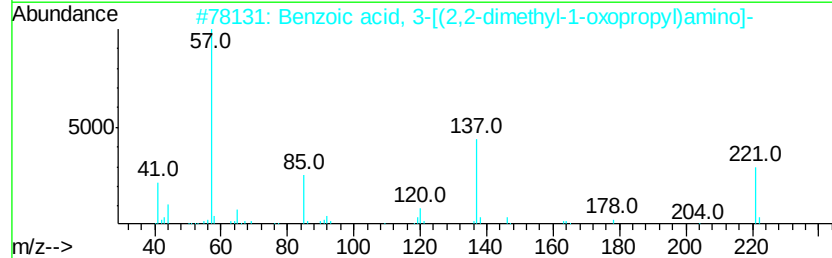
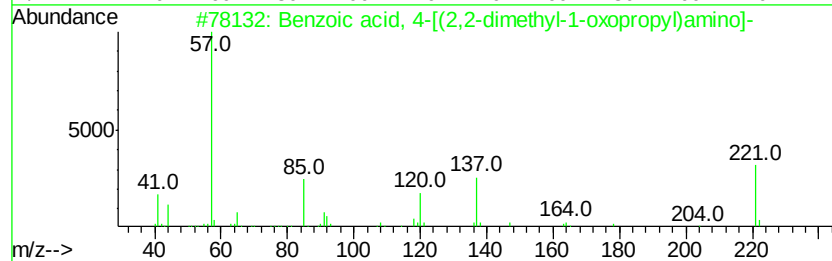
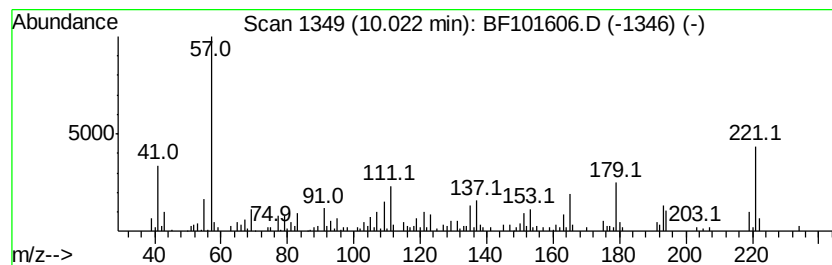
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown10.02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	2.77 ng	121988	Acenaphthene-d10	9.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzoic acid, 4-[(2,2-dimethyl-1...	221 C12H15N03	056619-97-7 14
2		Benzoic acid, 3-[(2,2-dimethyl-1...	221 C12H15N03	056619-96-6 14
3		Hexahydroxyindole, 4-[(4,5-dimeth...	221 C13H19N02	042434-76-4 12
4		Propanamide, N-(3-methoxy-2-meth...	221 C13H19N02	1000221-47-2 9
5		2-tert-Butoxycarbonylamino-3-(4-...	310 C14H18N2O6	086937-80-6 9



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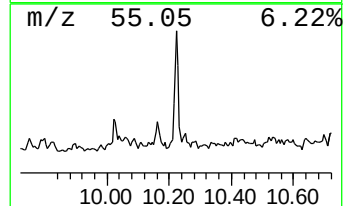
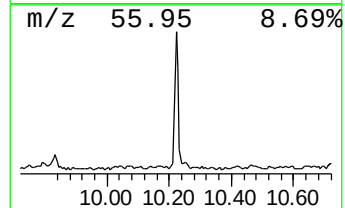
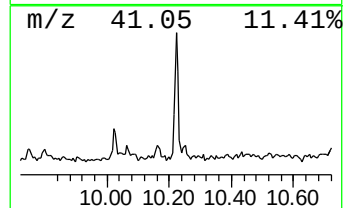
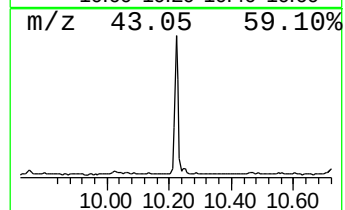
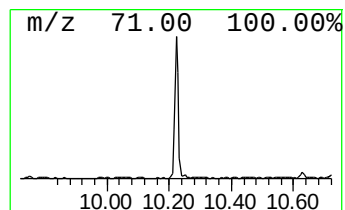
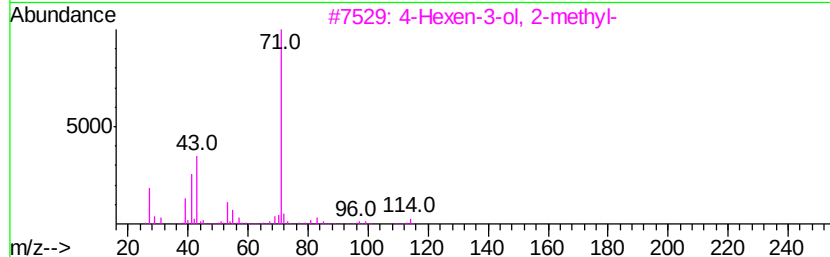
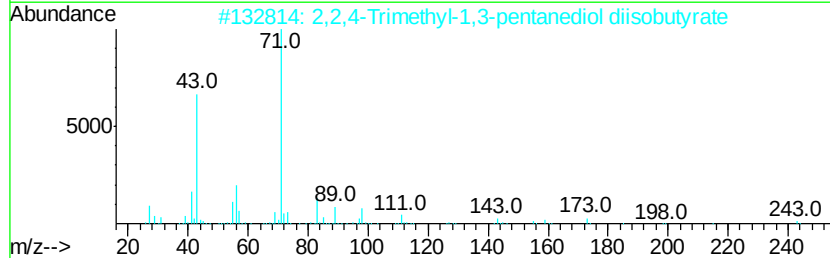
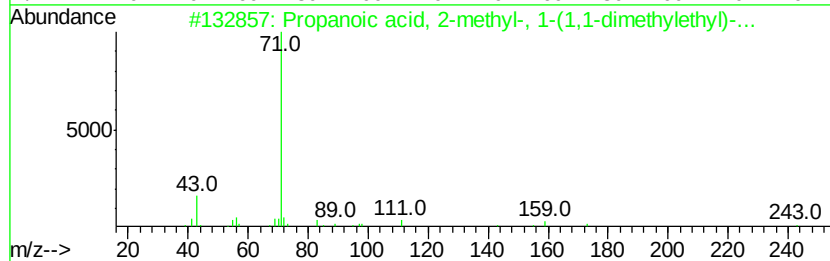
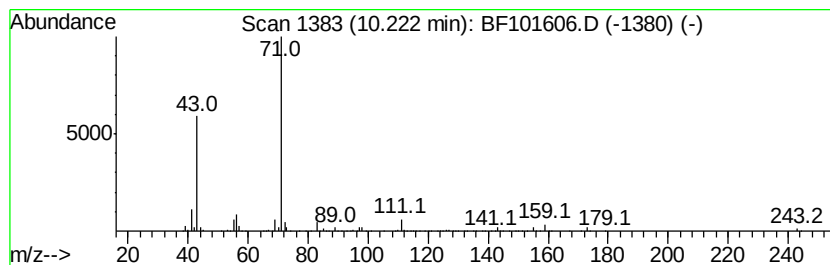
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Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.22	9.95 ng	437986	Acenaphthene-d10	9.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	91
2	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	78
3	4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	64
4	Propanoic acid, 2-methyl-, 1,2,3...	302	C15H26O6	014295-64-8	64
5	Fumaric acid, nonyl tetrahydrofu...	326	C18H30O5	1000330-58-3	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122117\
Data File : BF101606.D
Acq On : 21 Dec 2017 14:56
Operator : SJ/JU
Sample : I6966-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

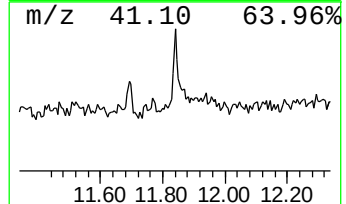
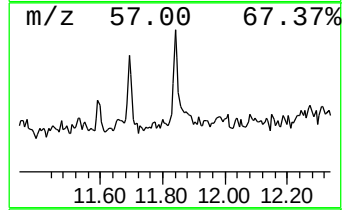
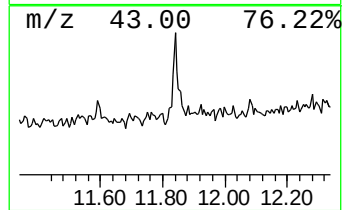
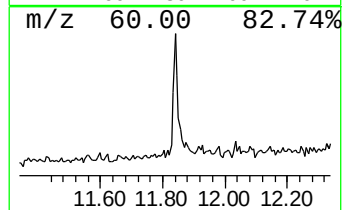
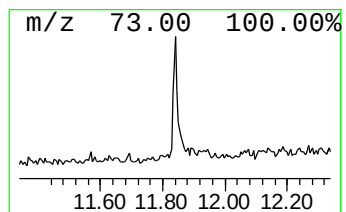
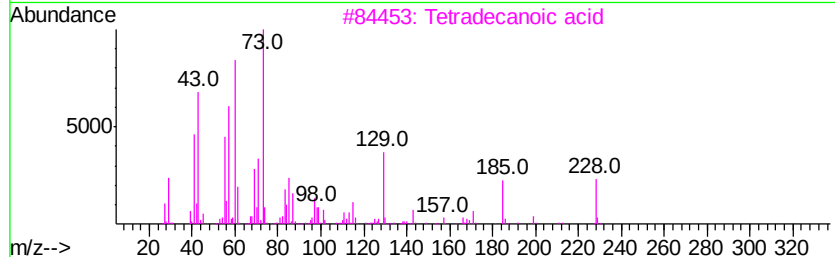
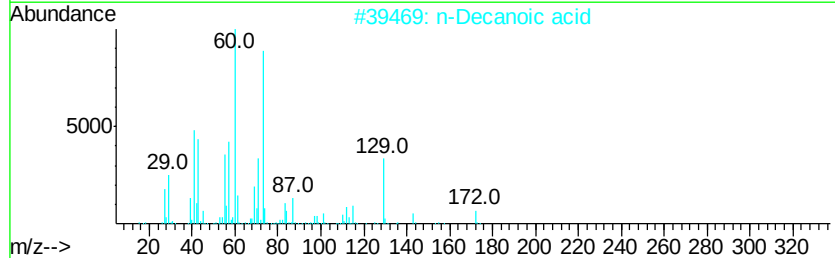
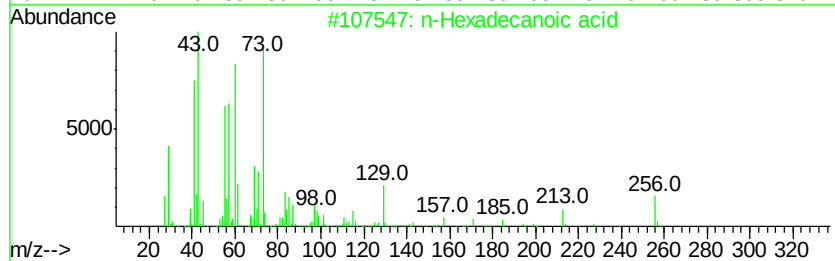
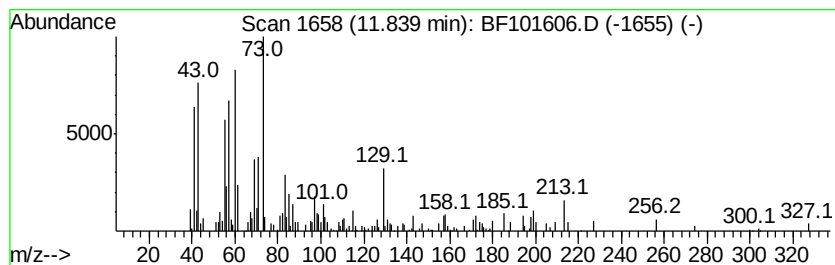
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.84	2.53 ng	99760	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	n-Decanoic acid	172	C10H20O2	000334-48-5	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122117\
Data File : BF101606.D
Acq On : 21 Dec 2017 14:56
Operator : SJ/JU
Sample : I6966-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

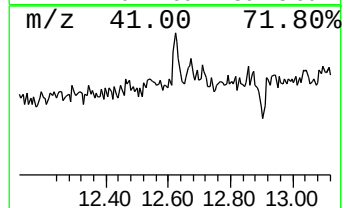
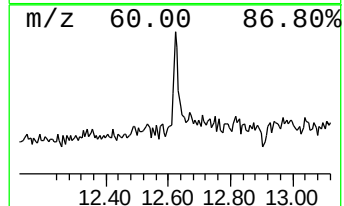
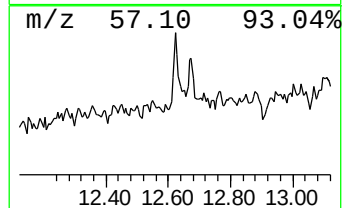
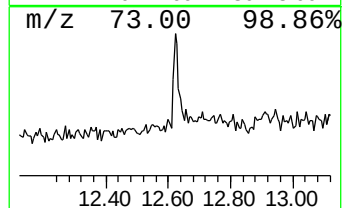
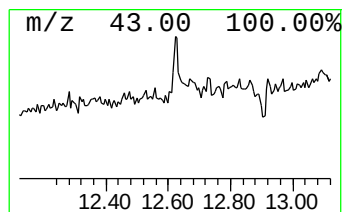
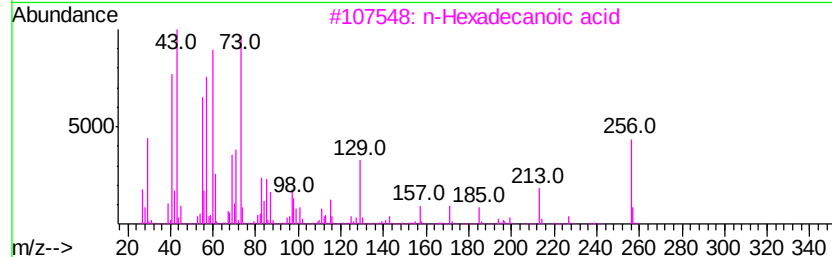
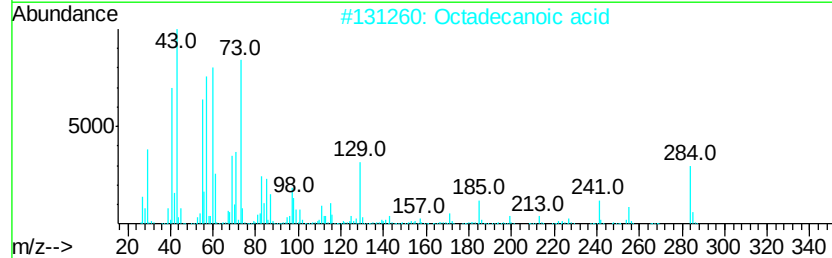
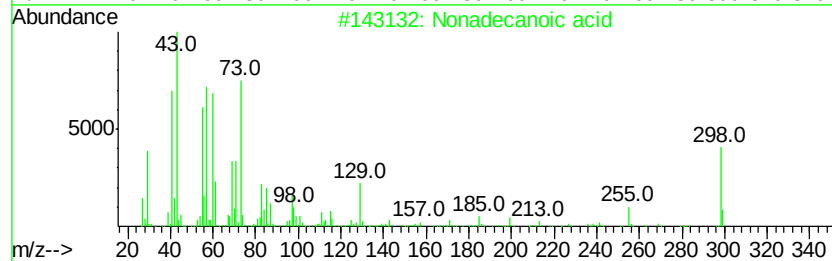
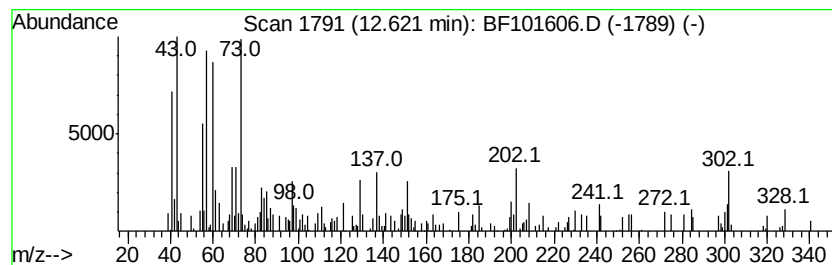
Instrument :
BNA_F
ClientSampleId :
DB-WATER

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	2.31 ng	91047	Phenanthrene-d10	11.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Nonadecanoic acid	298 C19H38O2	000646-30-0 94
2		Octadecanoic acid	284 C18H36O2	000057-11-4 86
3		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 59
4		Isopropyl palmitate	298 C19H38O2	000142-91-6 55
5		Pentadecanoic acid	242 C15H30O2	001002-84-2 42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122117\
Data File : BF101606.D
Acq On : 21 Dec 2017 14:56
Operator : SJ/JU
Sample : I6966-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DB-WATER

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	5.00	4.4	ng	174360	1	6.80	786564	20.0
unknown6.57	6.57	66.2	ng	2603550	1	6.80	786564	20.0
Phenol, 4-(1,1-di...	9.26	3.9	ng	171391	3	9.83	880347	20.0
unknown10.02	10.02	2.8	ng	121988	3	9.83	880347	20.0
Propanoic acid, 2...	10.22	9.9	ng	437986	3	9.83	880347	20.0
n-Hexadecanoic acid	11.84	2.5	ng	99760	4	11.32	787793	20.0
Nonadecanoic acid	12.62	2.3	ng	91047	4	11.32	787793	20.0