

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102317\
 Data File : BF099768.D
 Acq On : 23 Oct 2017 19:30
 Operator : SJ/JU
 Sample : I5950-10
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20170723-C-A-COMP2

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-BF102317.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	2.381	46	50	61	rVB	106501	161534	2.52%	0.417%
2	3.887	302	306	329	rBV	288848	456435	7.12%	1.178%
3	4.446	397	401	422	rVB	595695	738655	11.52%	1.907%
4	5.016	495	498	511	rBV	109971	146079	2.28%	0.377%
5	5.422	565	567	585	rVB	966948	1025840	16.00%	2.648%
6	5.598	592	597	601	rBV	130205	166458	2.60%	0.430%
7	6.210	698	701	709	rVB	97682	114339	1.78%	0.295%
8	6.445	738	741	745	rBV	592912	656348	10.24%	1.694%
9	6.575	759	763	767	rBV	2026545	2034482	31.73%	5.251%
10	6.804	798	802	808	rBV	598384	573005	8.94%	1.479%
11	6.863	809	812	820	rVV	105679	105096	1.64%	0.271%
12	6.957	824	828	837	rVB	2062020	2135557	33.30%	5.512%
13	7.128	854	857	864	rBV2	56995	89803	1.40%	0.232%
14	7.234	864	875	881	rBV3	218690	512828	8.00%	1.324%
15	7.334	888	892	895	rBV3	48003	71223	1.11%	0.184%
16	7.375	895	899	902	rVB	1561112	1529996	23.86%	3.949%
17	7.451	909	912	915	rBV	140801	111496	1.74%	0.288%
18	7.810	968	973	974	rBV	64486	78071	1.22%	0.202%
19	7.892	974	987	992	rVB2	318350	855854	13.35%	2.209%
20	8.116	1015	1025	1028	rVV2	4031249	6412613	100.00%	16.552%
21	8.163	1028	1033	1036	rVB	624496	592921	9.25%	1.530%
22	8.451	1078	1082	1090	rVB2	162640	189299	2.95%	0.489%
23	8.798	1137	1141	1145	rVV	1493896	1274877	19.88%	3.291%
24	8.898	1153	1158	1161	rVV	839293	739869	11.54%	1.910%
25	9.010	1173	1177	1181	rBV	153397	156800	2.45%	0.405%
26	9.163	1196	1203	1206	rVB	3116904	3160178	49.28%	8.157%
27	9.263	1217	1220	1223	rVB	308701	257488	4.02%	0.665%
28	9.316	1223	1229	1232	rBV	169766	185409	2.89%	0.479%
29	9.351	1232	1235	1240	rVV2	185896	220867	3.44%	0.570%
30	9.422	1244	1247	1252	rVV	89664	145829	2.27%	0.376%
31	9.498	1256	1260	1263	rVV	156503	175090	2.73%	0.452%
32	9.528	1263	1265	1269	rVB2	93392	91578	1.43%	0.236%
33	9.616	1277	1280	1282	rBV	78093	72834	1.14%	0.188%
34	9.651	1282	1286	1291	rVV2	177058	190625	2.97%	0.492%

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35	9.704	1291	1295	1298	rVV	246386	216252	3.37%	0.558%
36	9.816	1311	1314	1315	rBV	83639	77935	1.22%	0.201%
37	9.839	1315	1318	1321	rVV2	1001709	909094	14.18%	2.347%
38	9.875	1321	1324	1326	rVV	673093	557142	8.69%	1.438%
39	10.045	1349	1353	1357	rBV	809358	857633	13.37%	2.214%
40	10.357	1403	1406	1408	rBV	135574	103913	1.62%	0.268%
41	10.386	1408	1411	1415	rVB	346540	327877	5.11%	0.846%
42	10.539	1432	1437	1440	rBV4	100236	149030	2.32%	0.385%
43	10.604	1444	1448	1450	rBV2	141448	136288	2.13%	0.352%
44	10.639	1450	1454	1457	rVB	1637006	1638004	25.54%	4.228%
45	10.757	1471	1474	1477	rBV	81962	70348	1.10%	0.182%
46	10.804	1480	1482	1484	rVV	135279	117412	1.83%	0.303%
47	10.839	1484	1488	1491	rVV3	169581	268267	4.18%	0.692%
48	10.875	1491	1494	1496	rVV	167750	165038	2.57%	0.426%
49	10.898	1496	1498	1500	rVV	104001	86738	1.35%	0.224%
50	10.928	1500	1503	1504	rVV2	101014	122593	1.91%	0.316%
51	10.957	1506	1508	1510	rVV	83137	73738	1.15%	0.190%
52	10.992	1510	1514	1517	rVV3	607112	619423	9.66%	1.599%
53	11.022	1517	1519	1521	rVV	155181	129704	2.02%	0.335%
54	11.063	1524	1526	1530	rVB	82433	78831	1.23%	0.203%
55	11.145	1536	1540	1543	rBV	307975	278389	4.34%	0.719%
56	11.204	1547	1550	1552	rVV2	78109	81293	1.27%	0.210%
57	11.228	1552	1554	1557	rVV	90768	74054	1.15%	0.191%
58	11.333	1565	1572	1574	rVV	1011620	1037840	16.18%	2.679%
59	11.357	1574	1576	1579	rVV	891832	688241	10.73%	1.776%
60	11.569	1607	1612	1616	rVB2	90317	105495	1.65%	0.272%
61	11.786	1645	1649	1652	rBV	156931	190843	2.98%	0.493%
62	11.851	1658	1660	1668	rVB2	107312	124562	1.94%	0.322%
63	12.045	1690	1693	1699	rVB	330010	298240	4.65%	0.770%
64	12.545	1775	1778	1784	rVV	82644	88109	1.37%	0.227%
65	12.633	1788	1793	1800	rVV4	60026	75345	1.17%	0.194%
66	12.916	1836	1841	1844	rBV	2339627	2460012	38.36%	6.350%
67	13.974	2018	2021	2028	rVB	585490	532242	8.30%	1.374%
68	15.439	2263	2270	2281	rVB	455574	572281	8.92%	1.477%

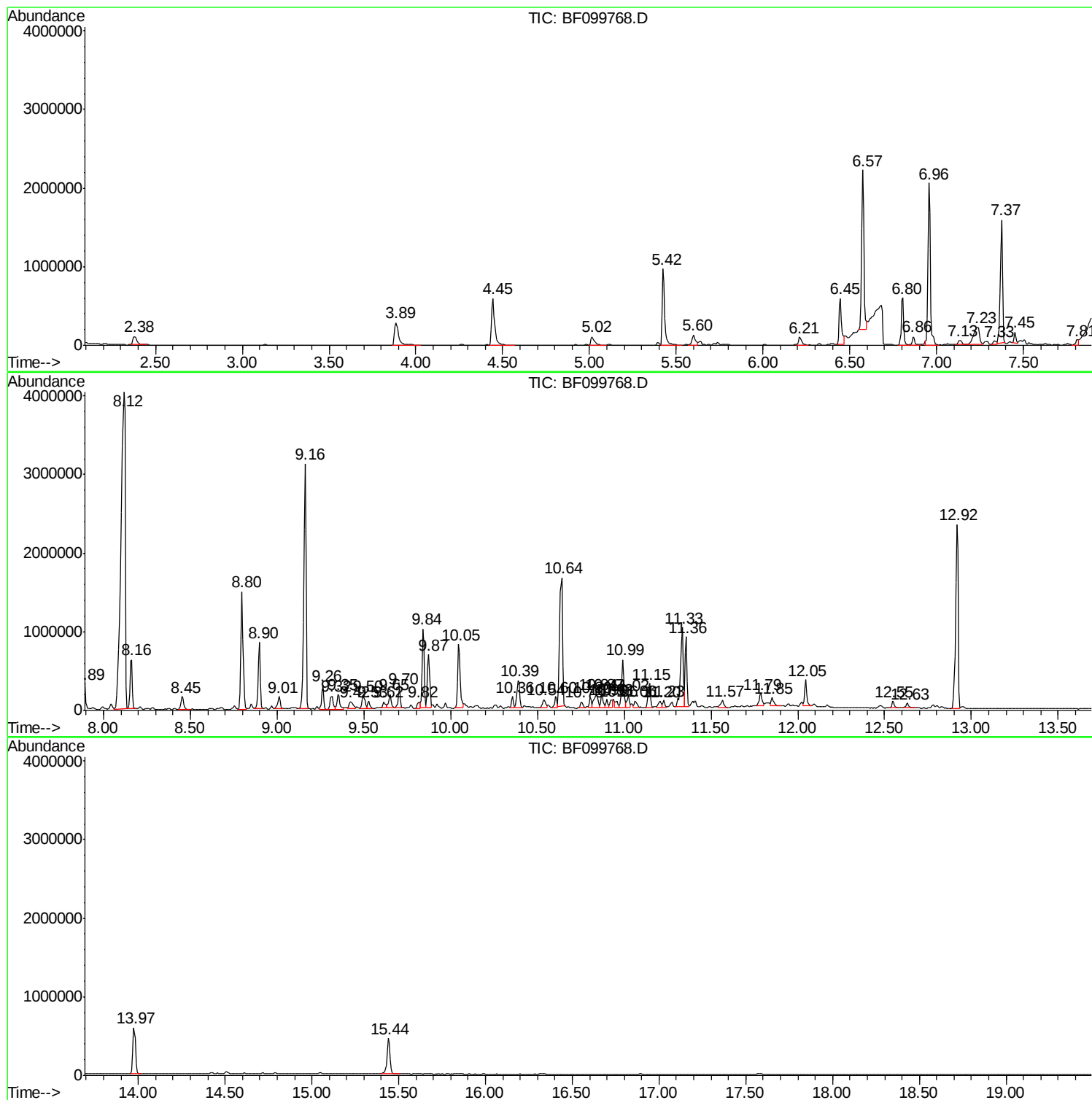
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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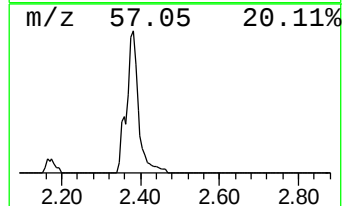
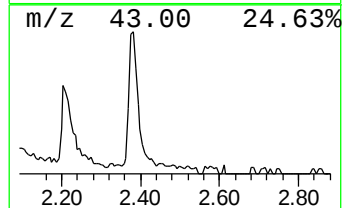
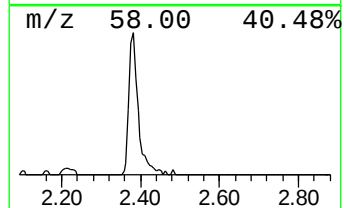
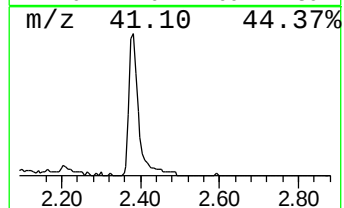
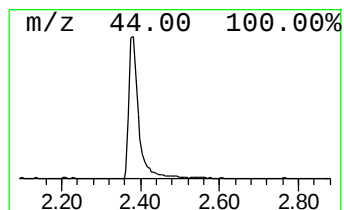
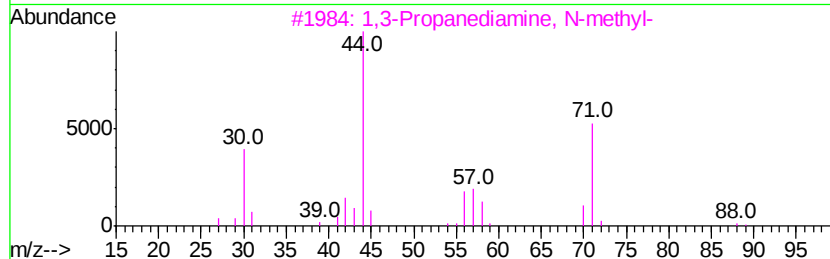
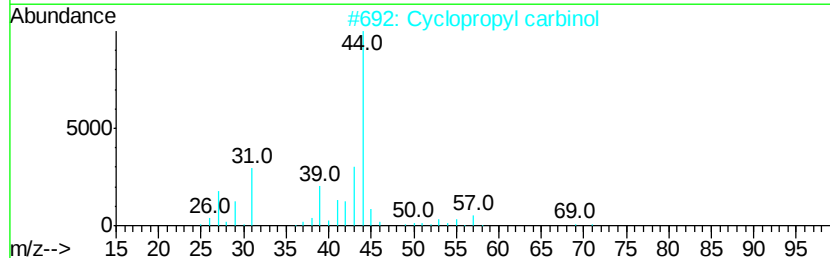
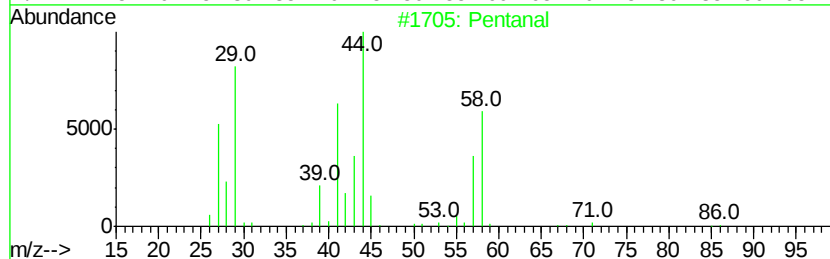
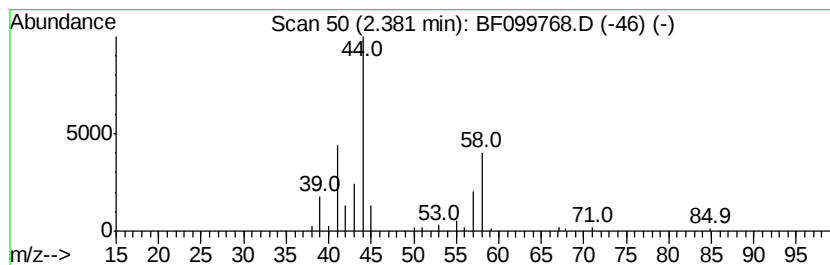
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	5.64 ng	161534	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	83
2	Cyclopropyl carbinol	72	C4H8O	002516-33-8	33
3	1,3-Propanediamine, N-methyl-	88	C4H12N2	006291-84-5	9
4	Glycidol	74	C3H6O2	000556-52-5	9
5	2-Propanamine	59	C3H9N	000075-31-0	7



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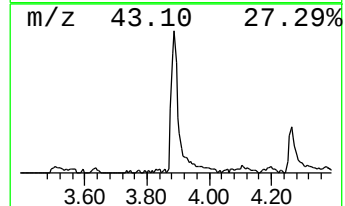
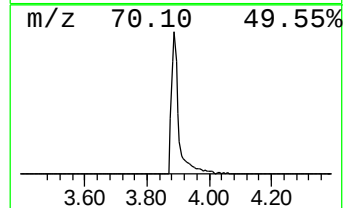
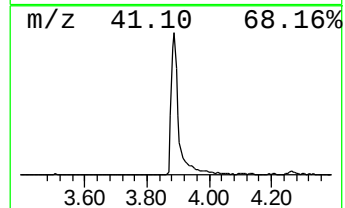
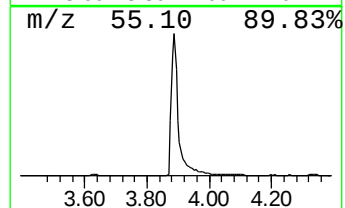
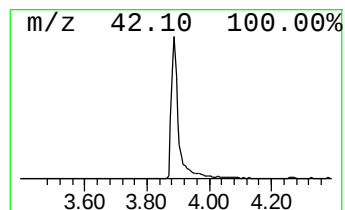
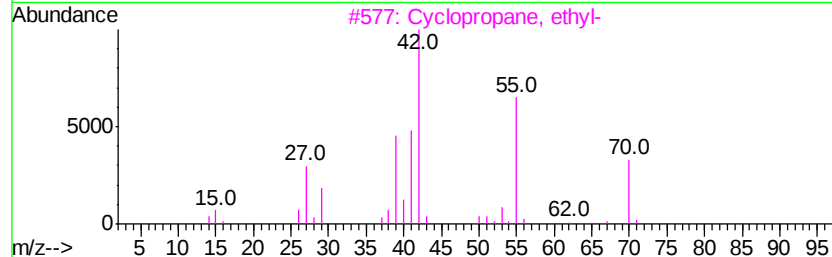
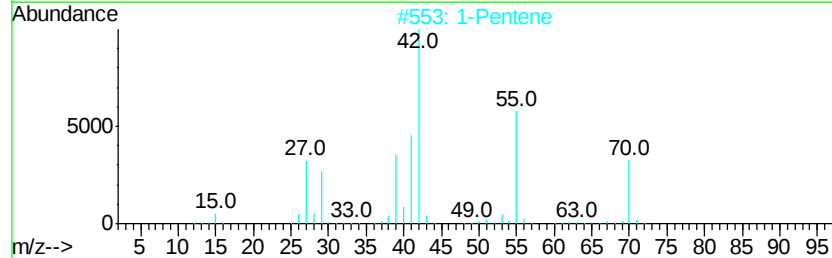
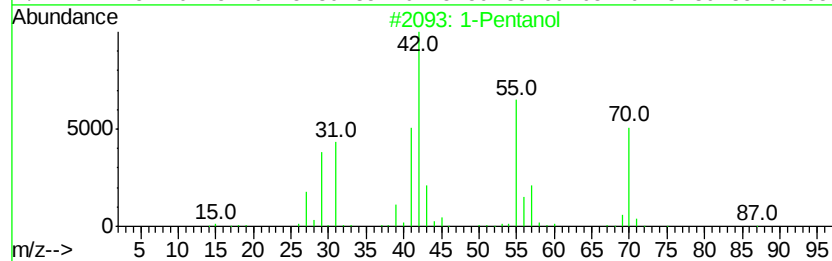
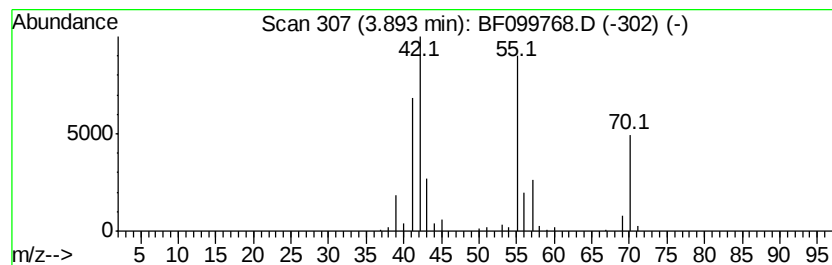
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1-Pentanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.89	15.93 ng	456435	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	90
2	1-Pentene	70	C5H10	000109-67-1	72
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
4	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	40
5	Cyclopropanecarboxaldehyde	70	C4H6O	001489-69-6	38



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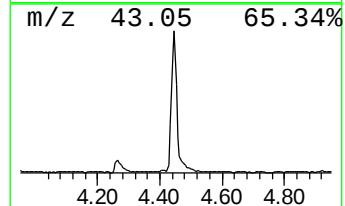
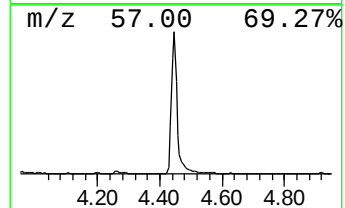
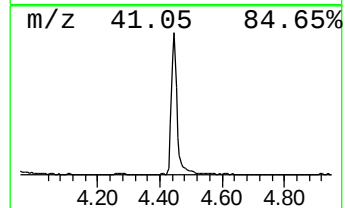
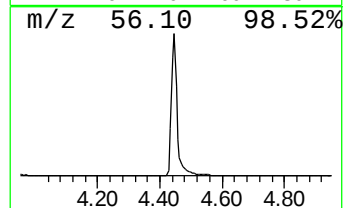
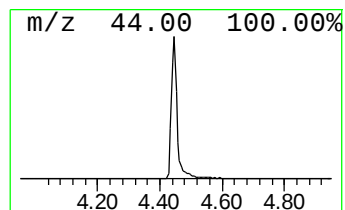
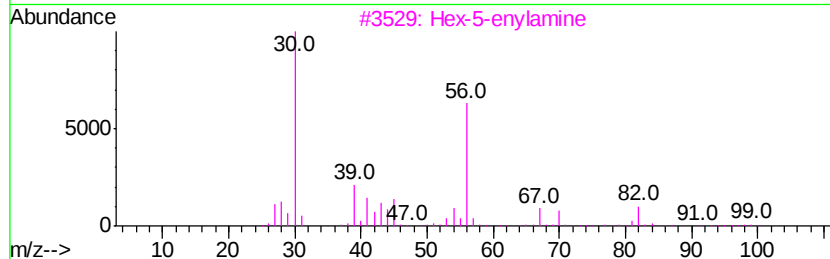
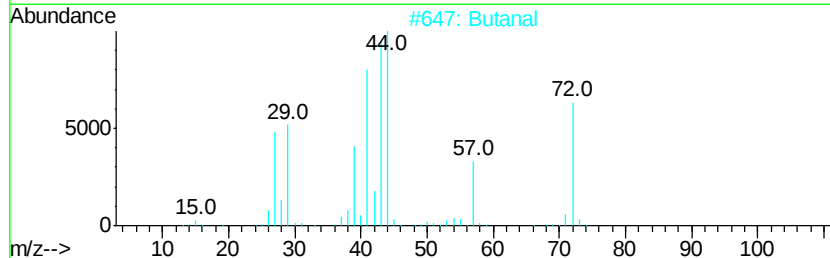
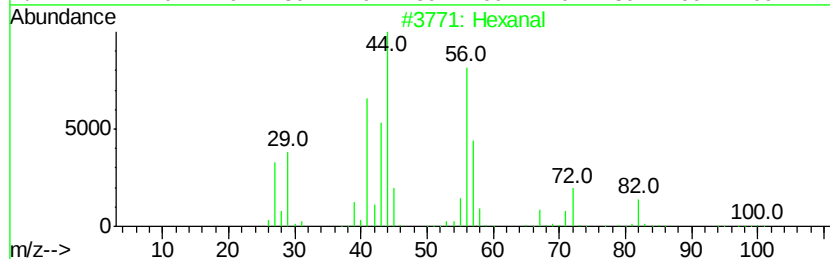
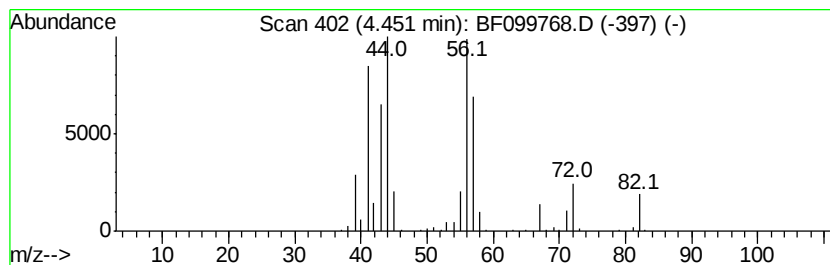
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	25.78 ng	738655	1,4-Dichlorobenzene-d4	6.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal		100	C6H12O	000066-25-1	90
2	Butanal		72	C4H8O	000123-72-8	35
3	Hex-5-enylamine		99	C6H13N	034825-70-2	23
4	Glutaraldehyde		100	C5H8O2	000111-30-8	23
5	Aziridine, 2-methyl-		57	C3H7N	000075-55-8	22



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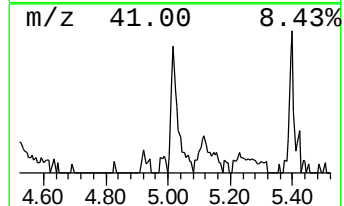
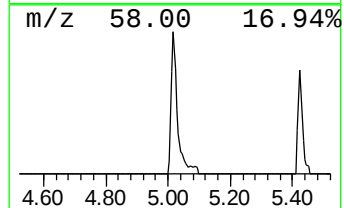
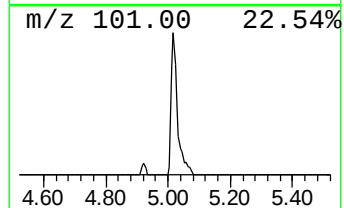
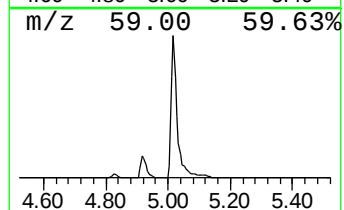
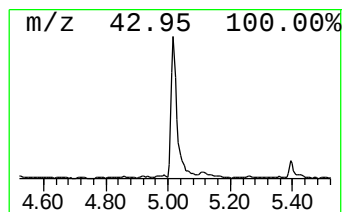
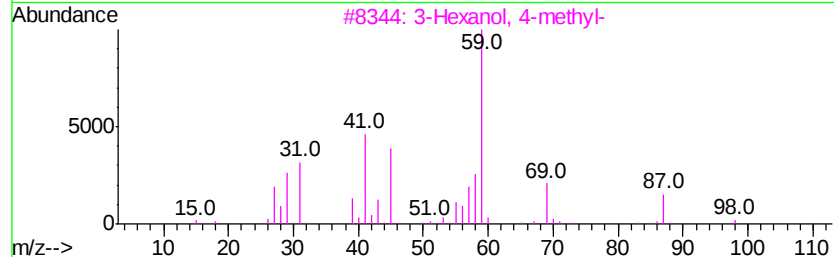
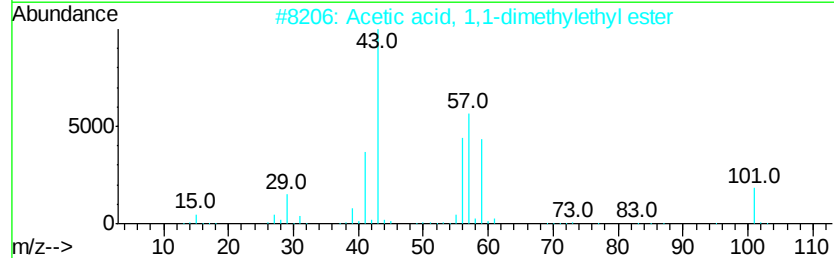
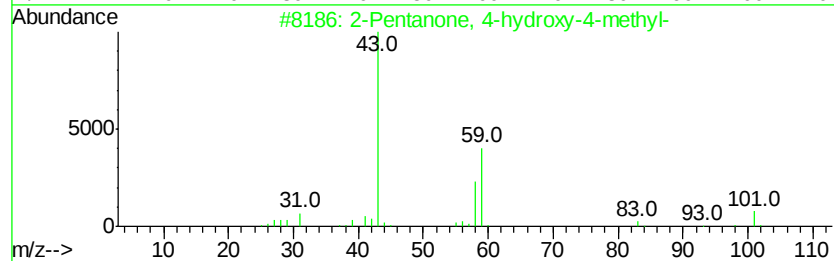
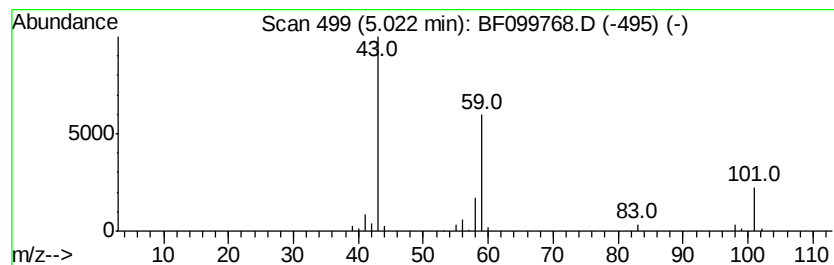
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	5.10 ng	146079	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	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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ClientSampleId :
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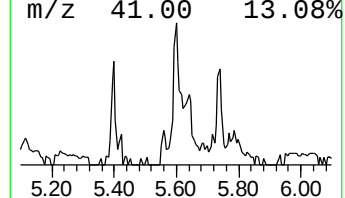
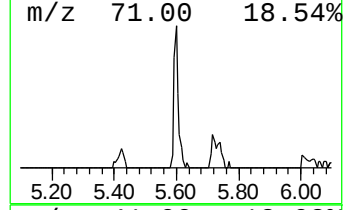
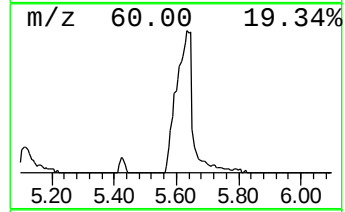
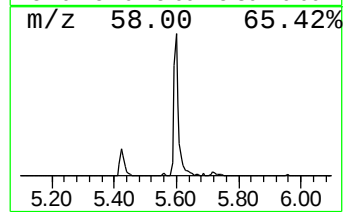
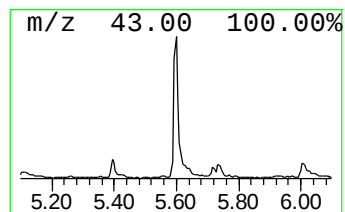
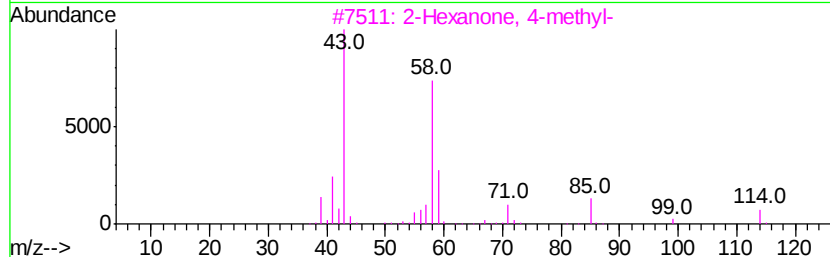
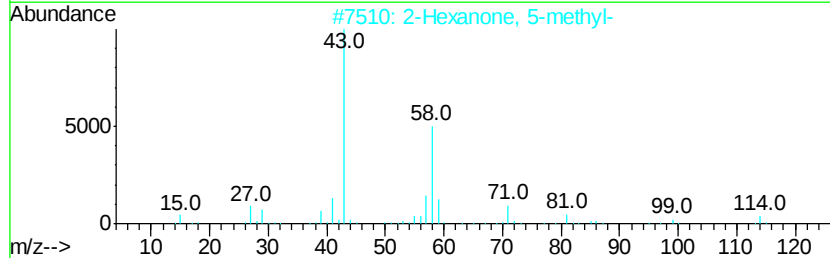
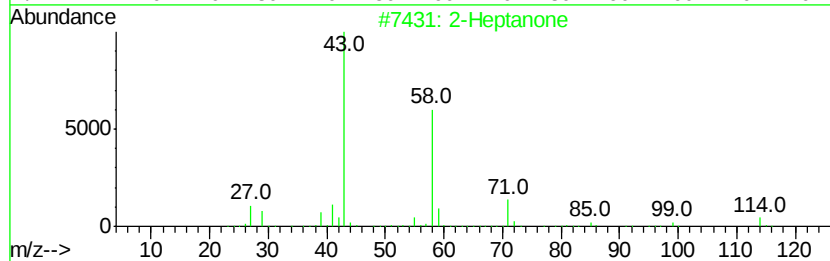
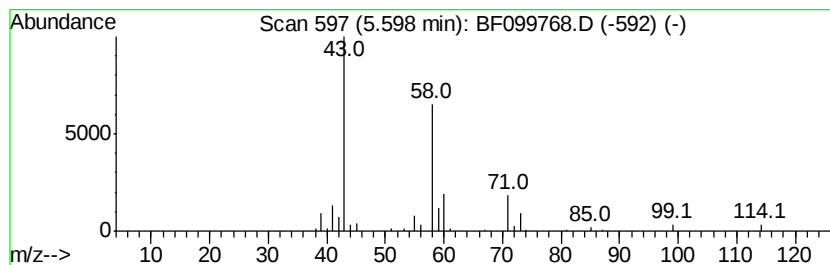
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Heptanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	5.81 ng	166458	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Heptanone	114	C7H14O	000110-43-0	68
2		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	53
3		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	38
4		Pentanal, 2-methyl-	100	C6H12O	000123-15-9	37
5		2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	33



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102317\
Data File : BF099768.D
Acq On : 23 Oct 2017 19:30
Operator : SJ/JU
Sample : I5950-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
20170723-C-A-COMP2

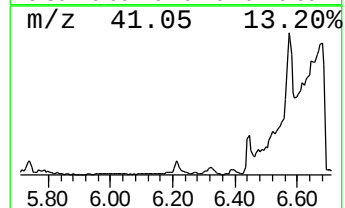
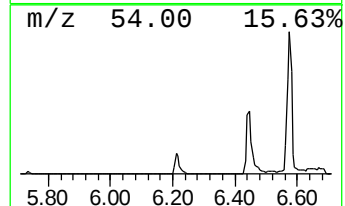
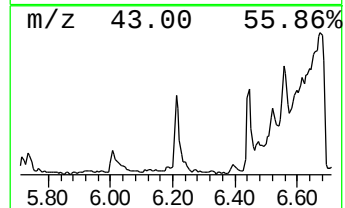
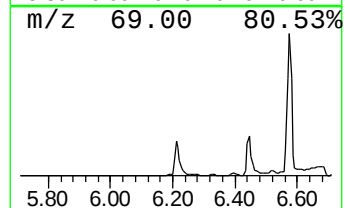
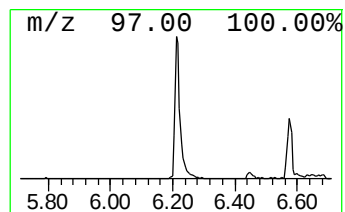
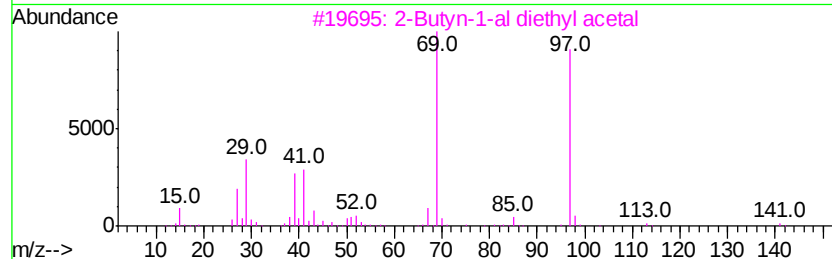
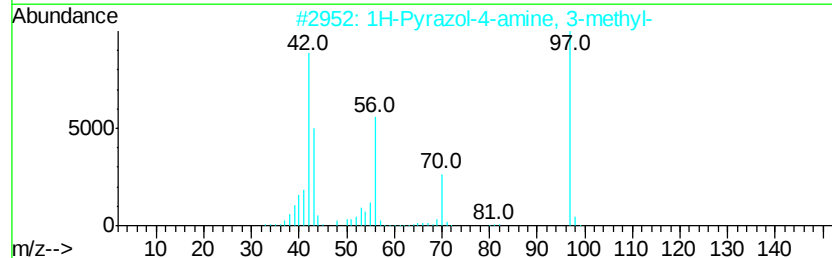
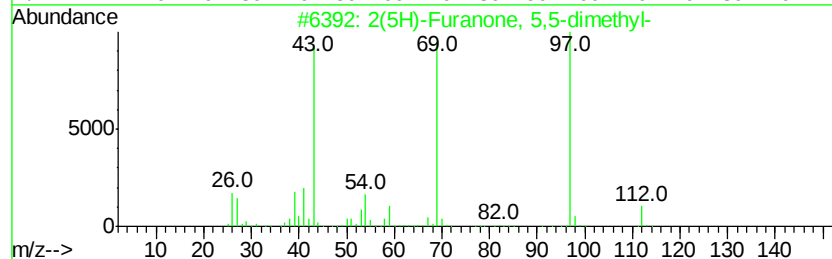
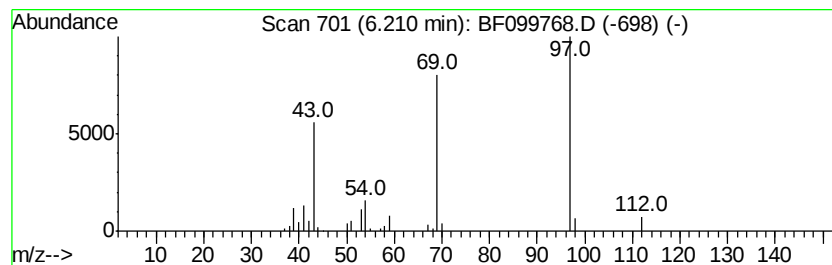
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2(5H)-Furanone, 5,5-dimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.21	3.99 ng	114339	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	64
2		1H-Pyrazol-4-amine, 3-methyl-	97	C4H7N3	1000338-28-2	43
3		2-Butyn-1-ol diethyl acetal	142	C8H14O2	002806-97-5	40
4		3-Butyn-2-ol, 2-methyl-	84	C5H8O	000115-19-5	38
5		1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102317\
Data File : BF099768.D
Acq On : 23 Oct 2017 19:30
Operator : SJ/JU
Sample : I5950-10
Misc :
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Instrument :
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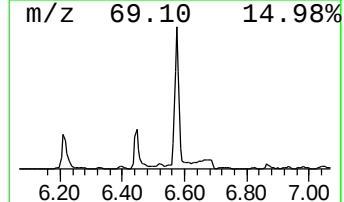
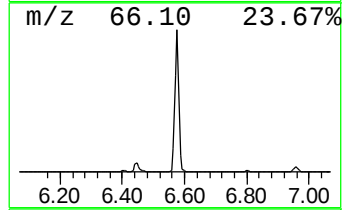
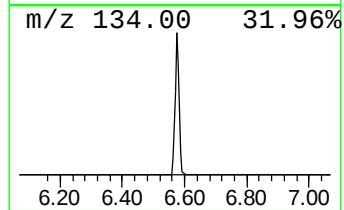
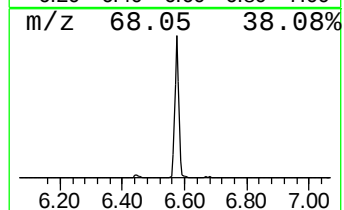
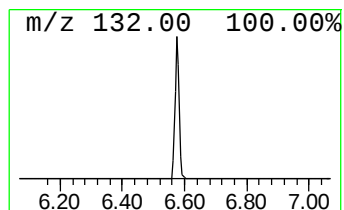
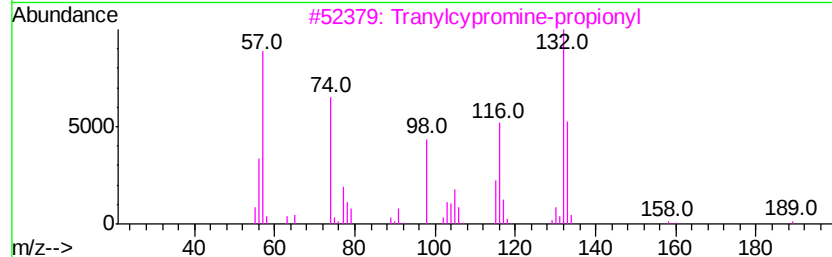
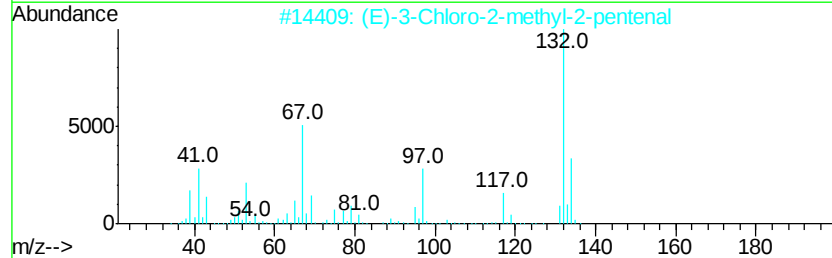
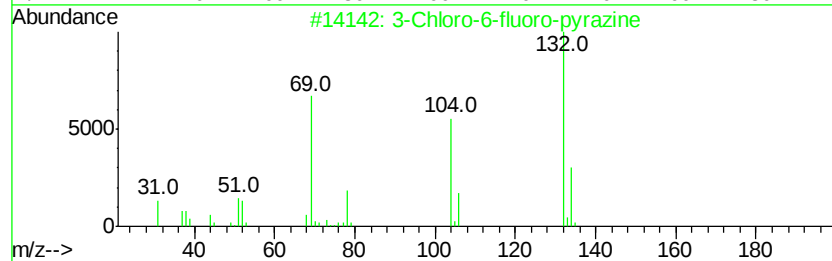
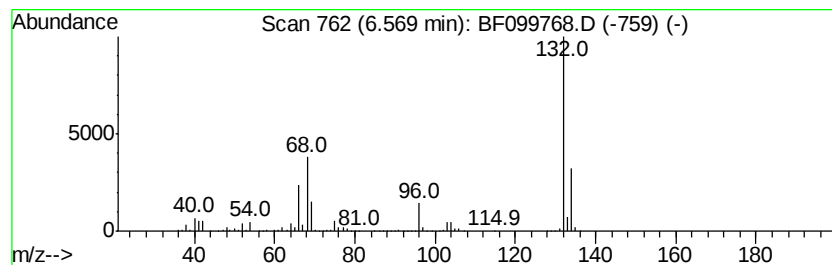
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	71.01 ng	2034480	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	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102317\
Data File : BF099768.D
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Operator : SJ/JU
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Misc :
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Instrument :
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ClientSampleId :
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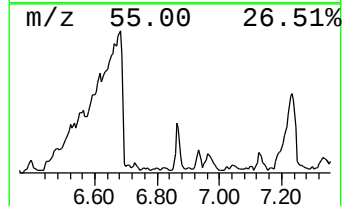
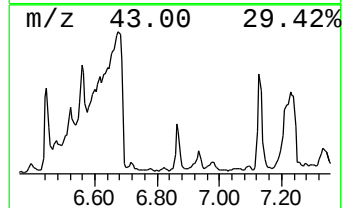
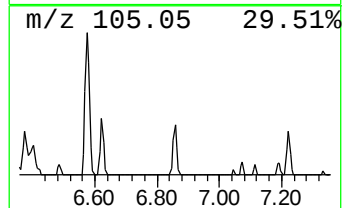
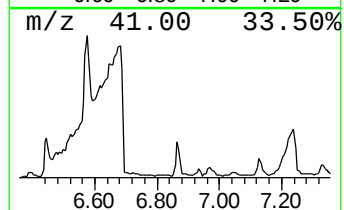
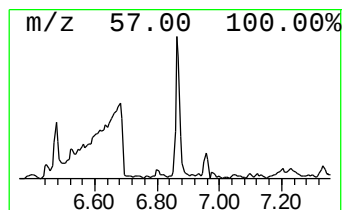
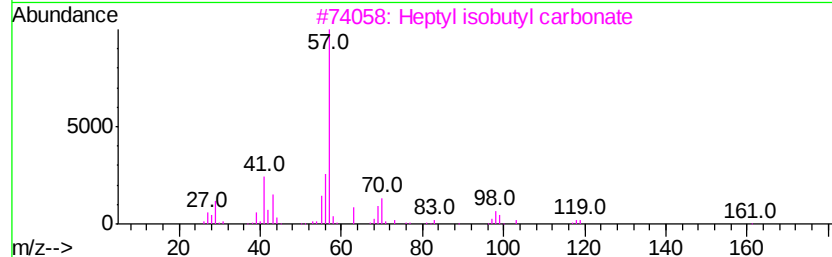
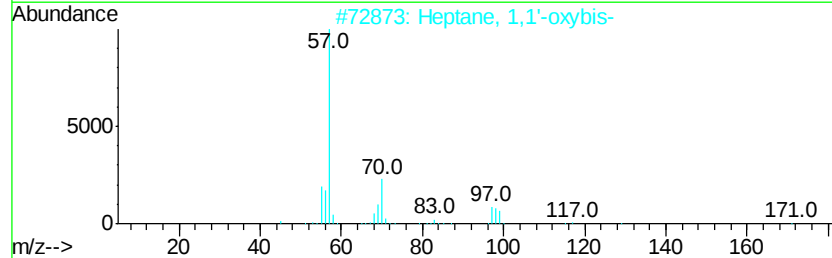
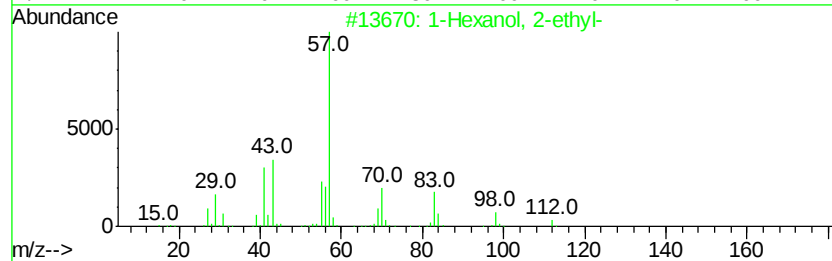
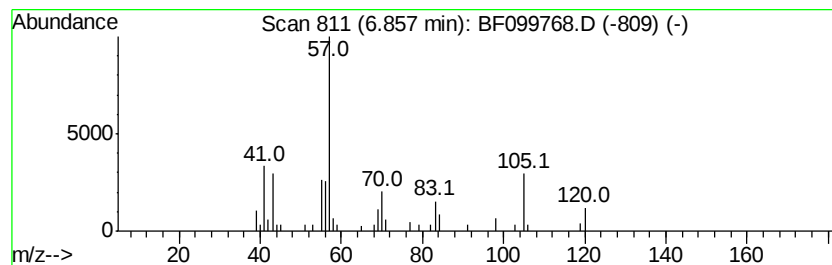
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.86	3.67 ng	105096	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102317\
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Operator : SJ/JU
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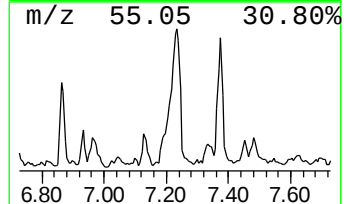
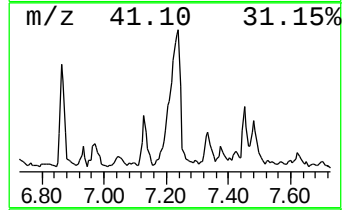
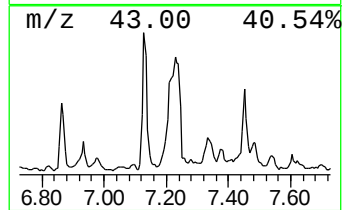
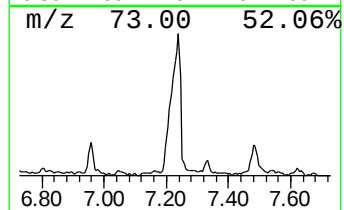
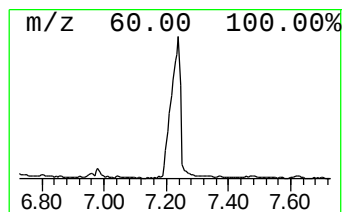
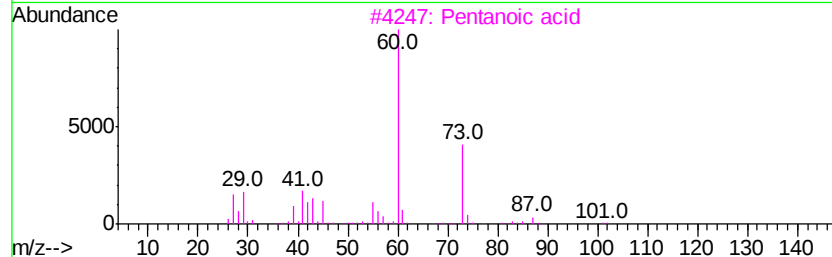
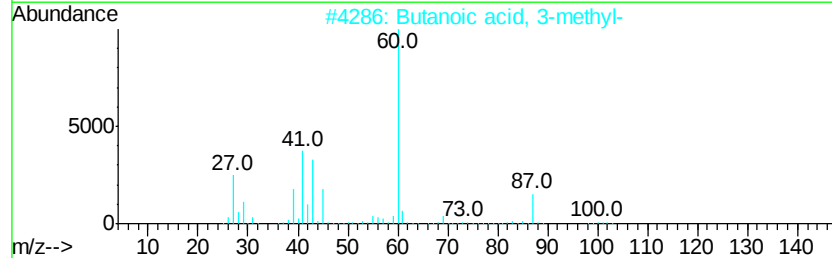
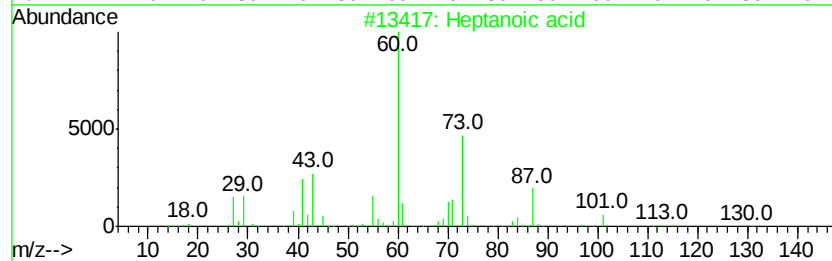
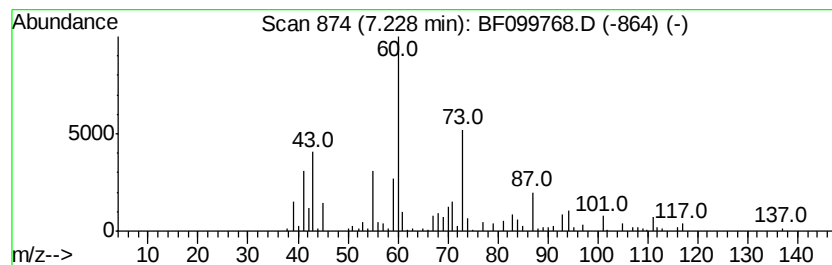
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	17.90 ng	512828	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptanoic acid	130	C7H14O2	000111-14-8	64
2		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	58
3		Pentanoic acid	102	C5H10O2	000109-52-4	50
4		Hexanoic acid	116	C6H12O2	000142-62-1	50
5		Octanoic acid	144	C8H16O2	000124-07-2	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102317\
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Operator : SJ/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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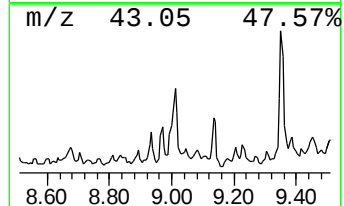
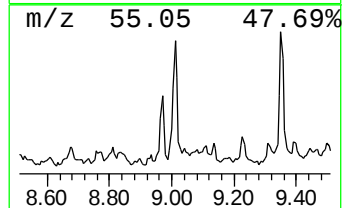
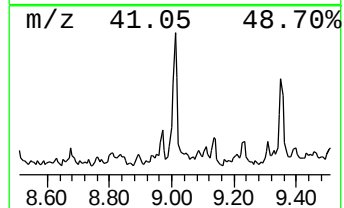
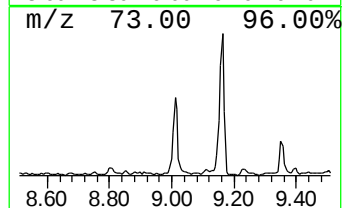
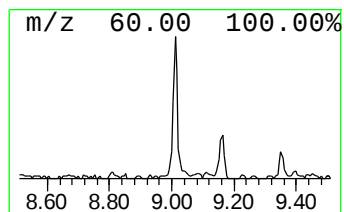
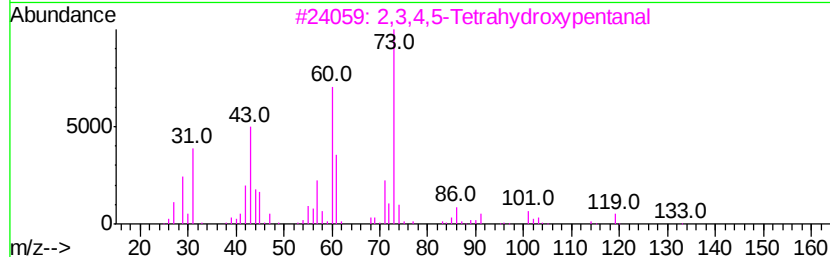
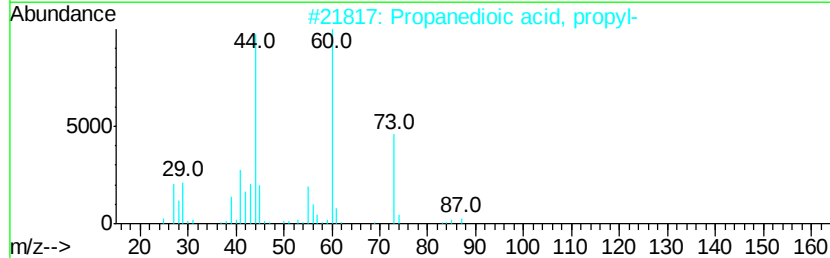
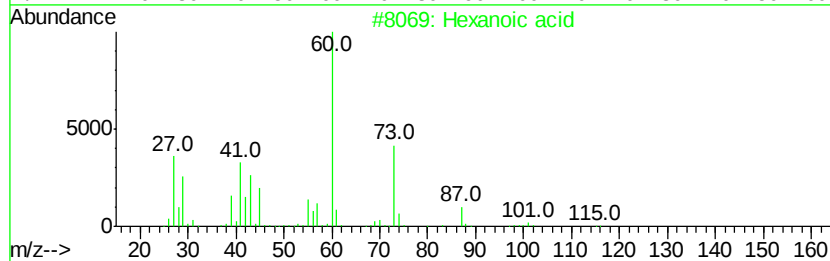
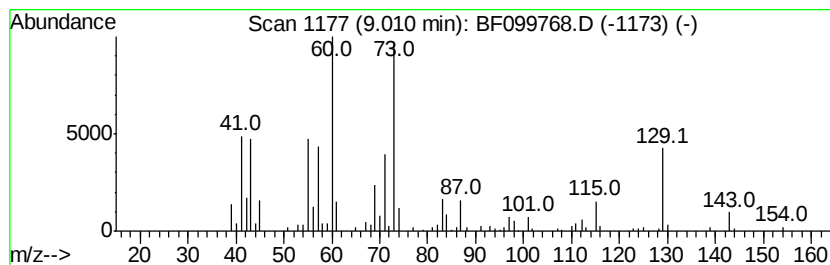
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.01	3.45 ng	156800	Acenaphthene-d10	9.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid	116	C6H12O2	000142-62-1	38
2			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	38
3			2,3,4,5-Tetrahydroxypentanal	150	C5H10O5	053106-52-8	38
4			Heptanoic acid	130	C7H14O2	000111-14-8	38
5			Octanoic acid	144	C8H16O2	000124-07-2	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102317\
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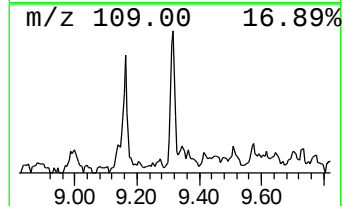
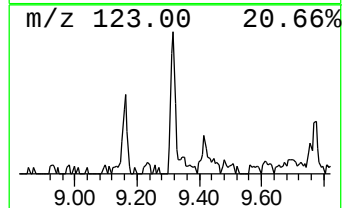
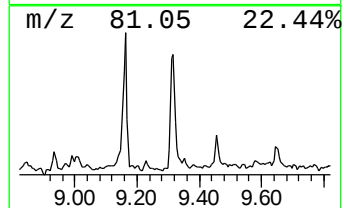
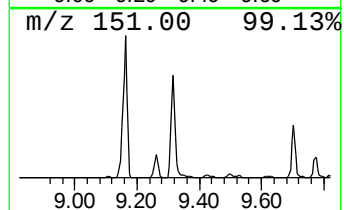
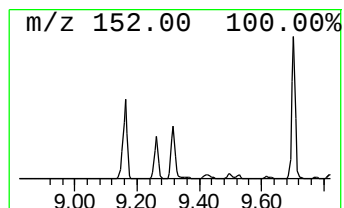
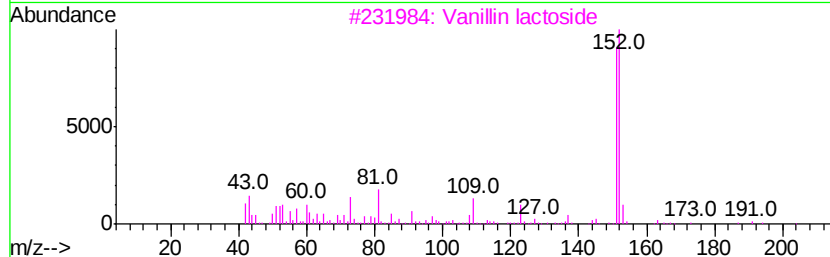
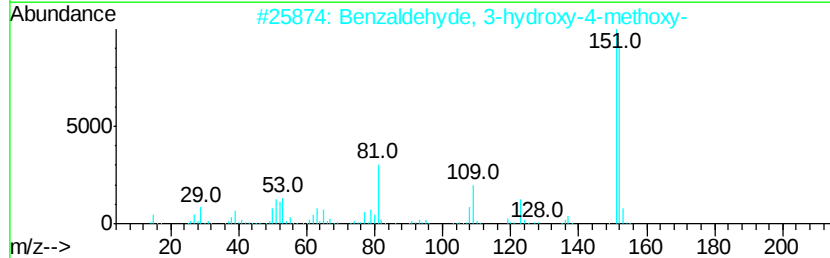
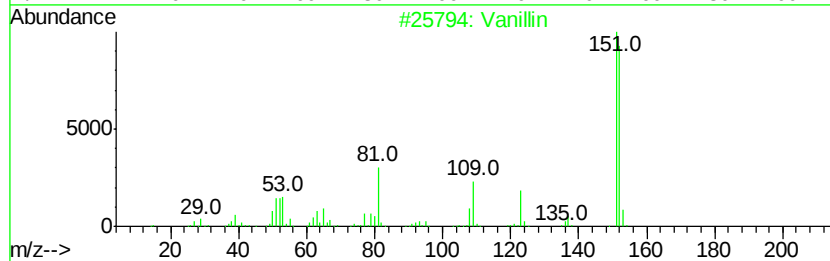
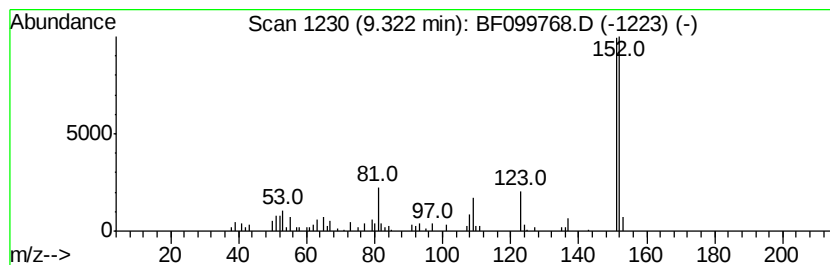
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Vanillin Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.32	4.08 ng	185409	Acenaphthene-d10	9.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vanillin	152	C8H8O3	000121-33-5	97
2		Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	94
3		Vanillin lactoside	476	C20H28O13	1000129-94-7	83
4		Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	64
5		Benzaldehyde, 3-(chloroacetoxy)-...	228	C10H9ClO4	066267-38-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102317\
Data File : BF099768.D
Acq On : 23 Oct 2017 19:30
Operator : SJ/JU
Sample : I5950-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20170723-C-A-COMP2

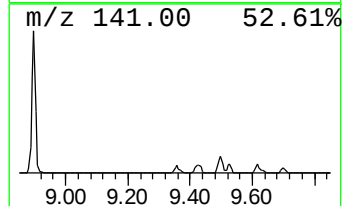
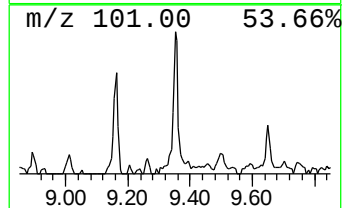
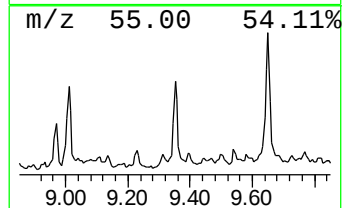
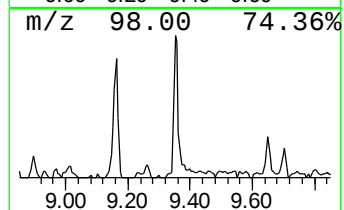
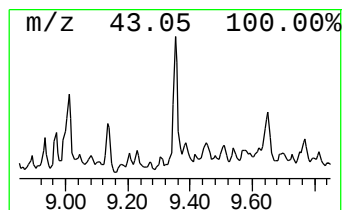
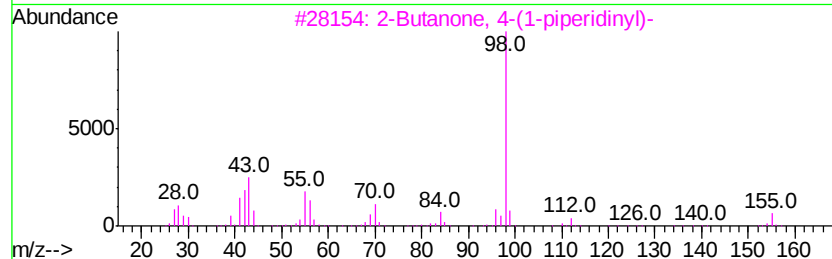
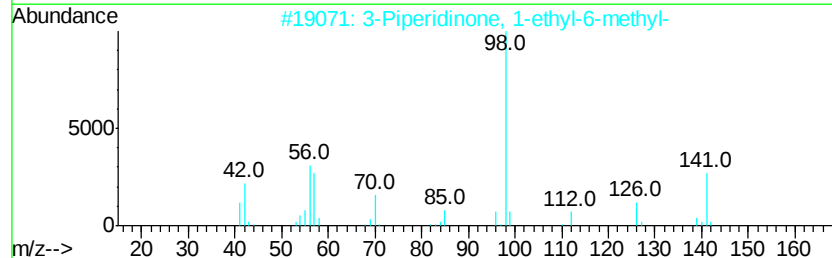
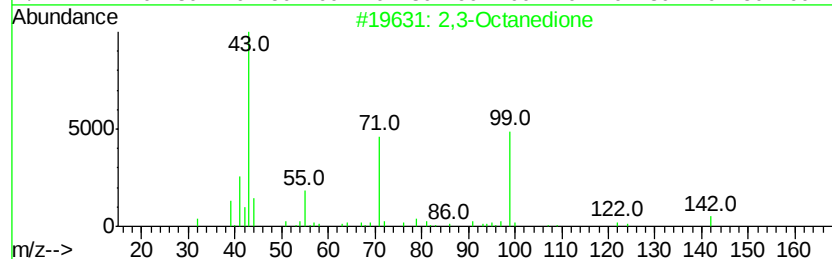
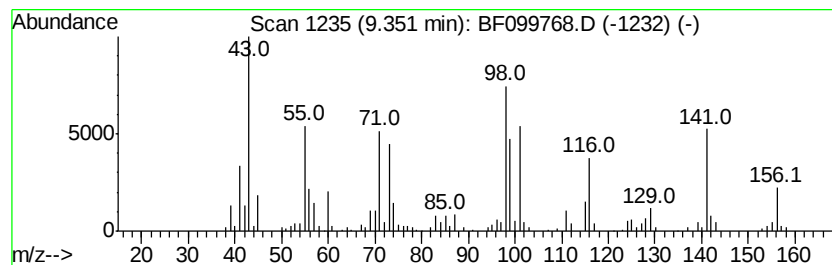
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown9.35 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.35	4.86 ng	220867	Acenaphthene-d10	9.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Octanedione	142	C8H14O2	000585-25-1	25
2			3-Piperidinone, 1-ethyl-6-methyl-	141	C8H15NO	043152-94-9	14
3			2-Butanone, 4-(1-piperidinyl)-	155	C9H17NO	016635-03-3	11
4			2-Pyrrolidinone, 3-hydroxy-3,4-d...	129	C6H11NO2	1000196-87-3	11
5			Thiazole, 4,5-dihydro-4-methyl-2...	116	C4H8N2S	010416-81-6	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102317\
Data File : BF099768.D
Acq On : 23 Oct 2017 19:30
Operator : SJ/JU
Sample : I5950-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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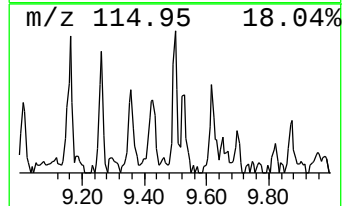
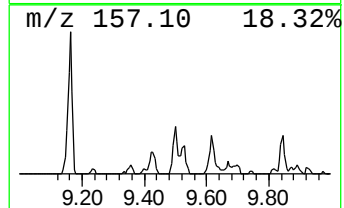
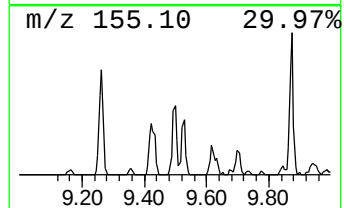
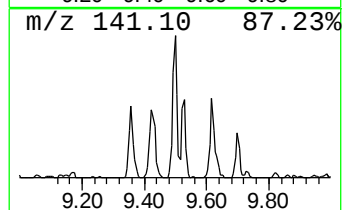
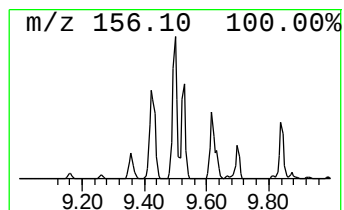
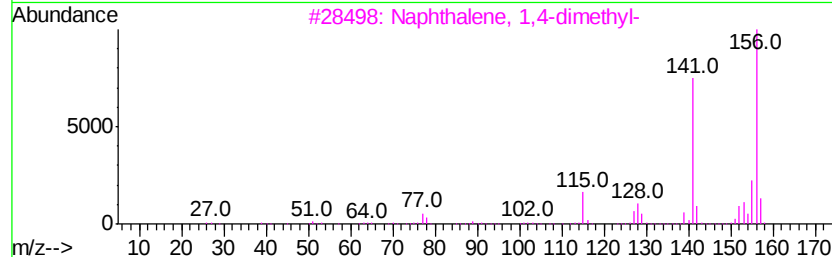
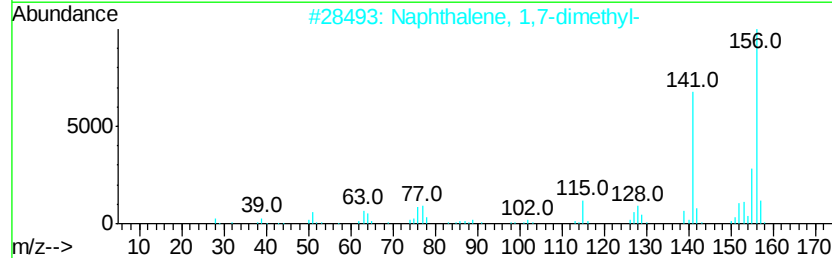
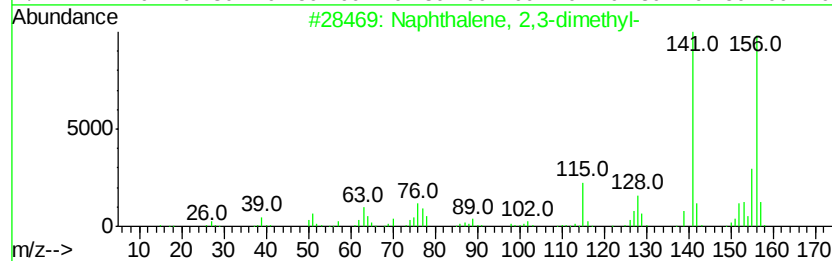
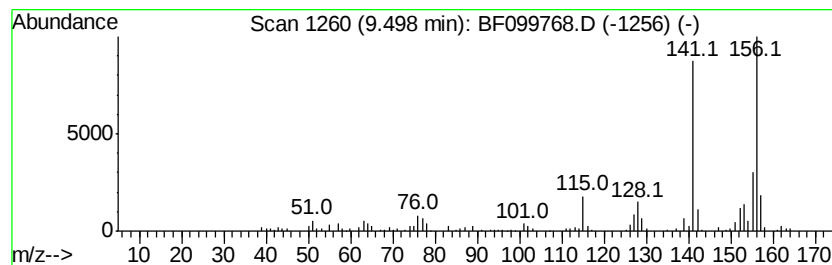
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Naphthalene, 2,3-dimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	3.85 ng	175090	Acenaphthene-d10	9.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	95



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102317\
Data File : BF099768.D
Acq On : 23 Oct 2017 19:30
Operator : SJ/JU
Sample : I5950-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

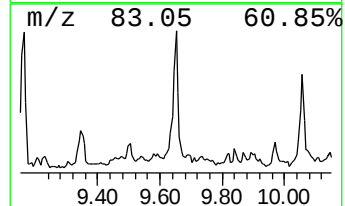
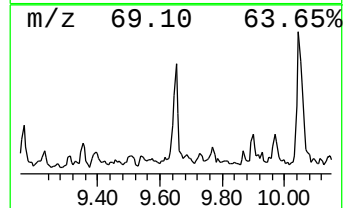
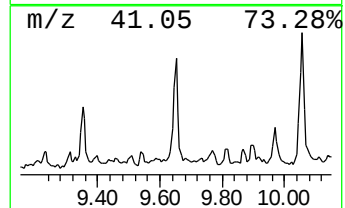
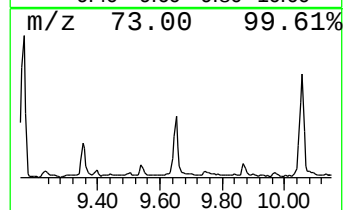
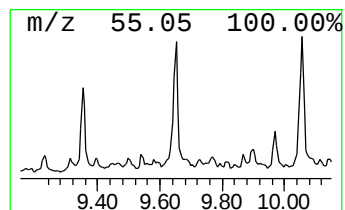
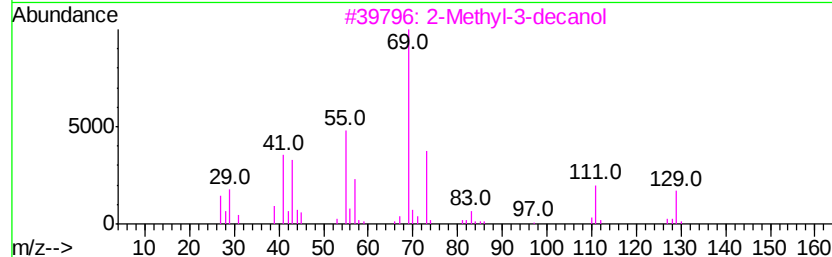
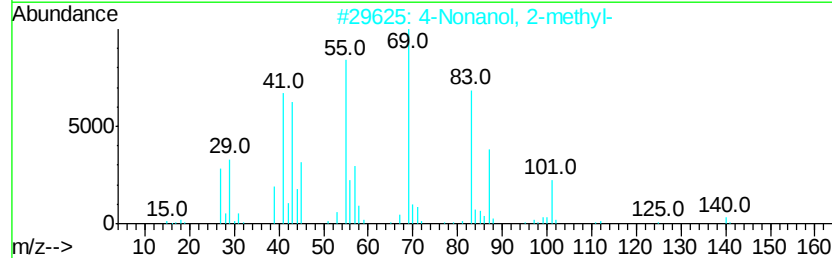
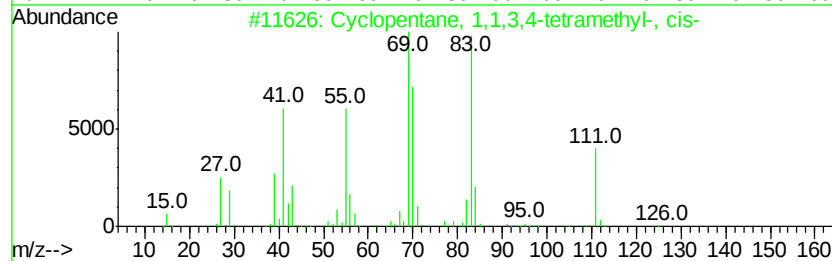
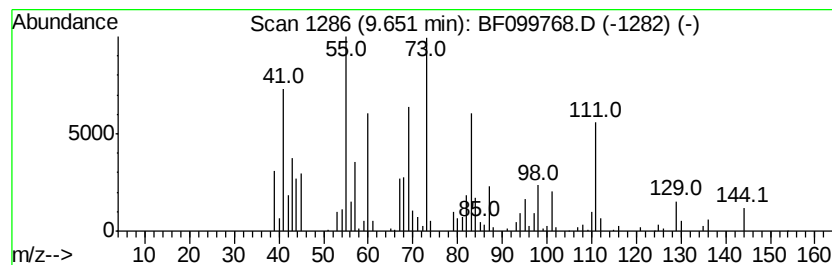
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown9.65 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.65	4.19 ng	190625	Acenaphthene-d10	9.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	053907-60-1	30
2	4-Nonanol, 2-methyl-	158	C10H22O	026533-31-3	22
3	2-Methyl-3-decanol	172	C11H24O	083909-79-9	22
4	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	22
5	Ethanol, 2-(cyclohexyloxy)-	144	C8H16O2	001817-88-5	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102317\
Data File : BF099768.D
Acq On : 23 Oct 2017 19:30
Operator : SJ/JU
Sample : I5950-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

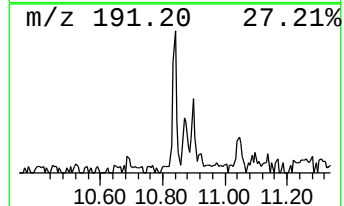
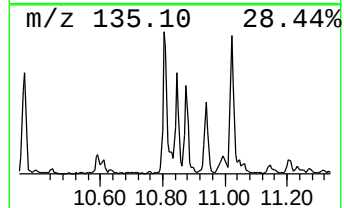
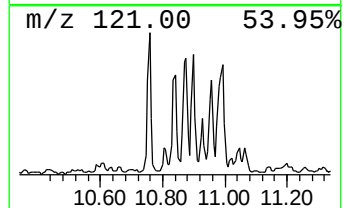
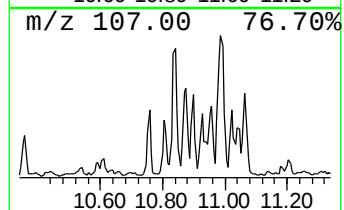
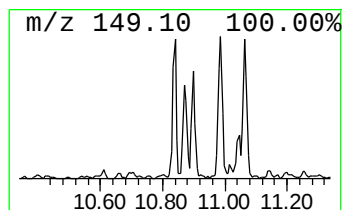
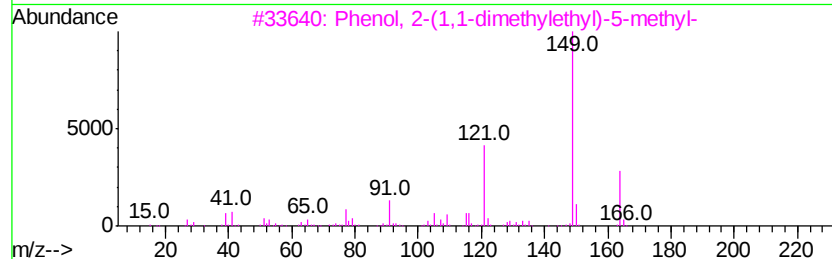
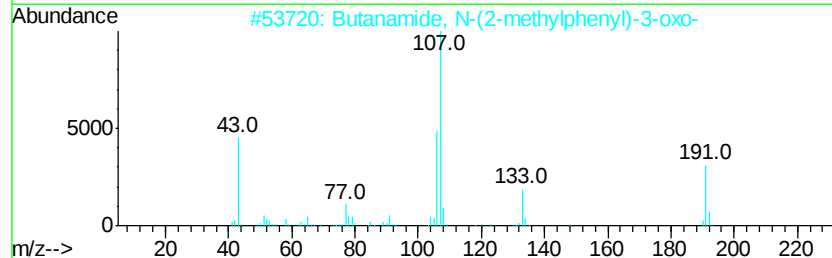
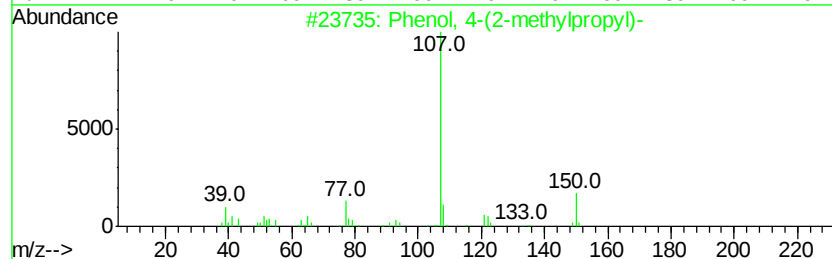
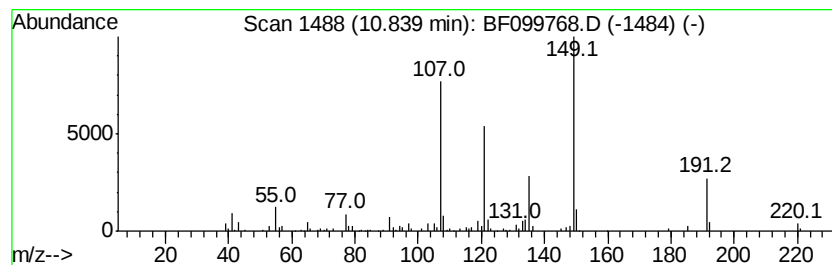
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown10.84 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.84	5.17 ng	268267	Phenanthrene-d10	11.33		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4-(2-methylpropyl)-	150	C10H14O	004167-74-2	38
2		Butanamide, N-(2-methylphenyl)-3...	191	C11H13NO2	000093-68-5	38
3		Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	35
4		Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	35
5		Butanamide, N-(4-methylphenyl)-3...	191	C11H13NO2	002415-85-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102317\
Data File : BF099768.D
Acq On : 23 Oct 2017 19:30
Operator : SJ/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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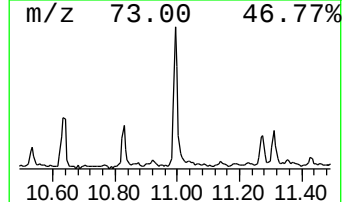
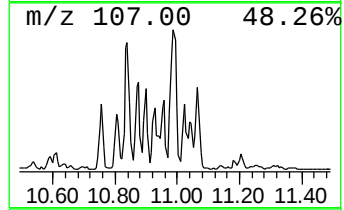
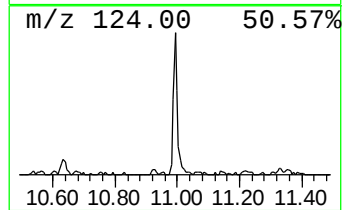
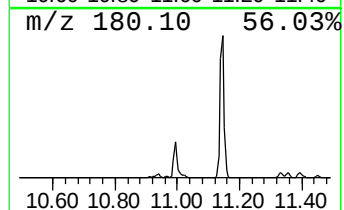
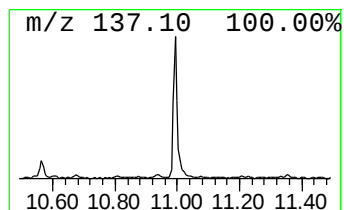
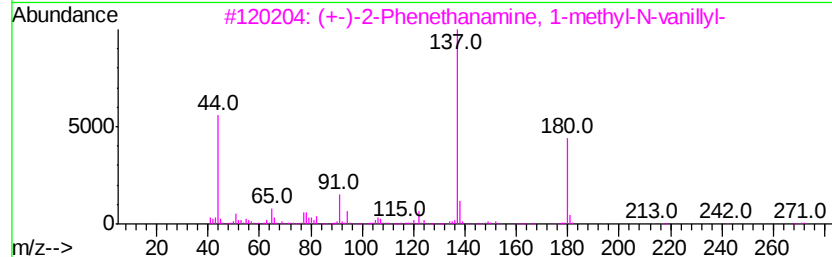
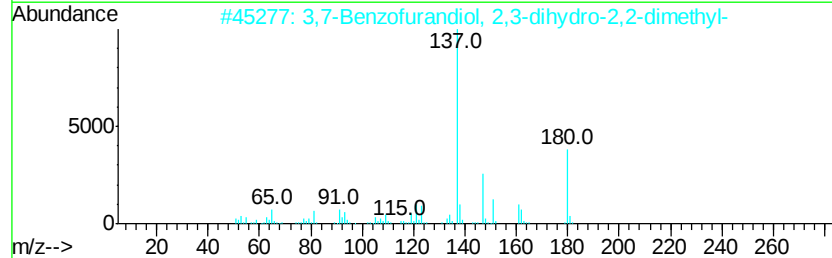
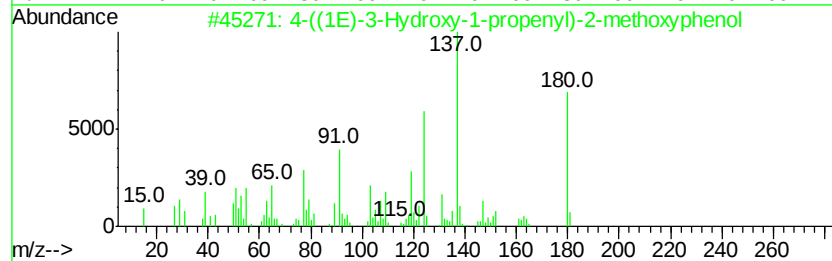
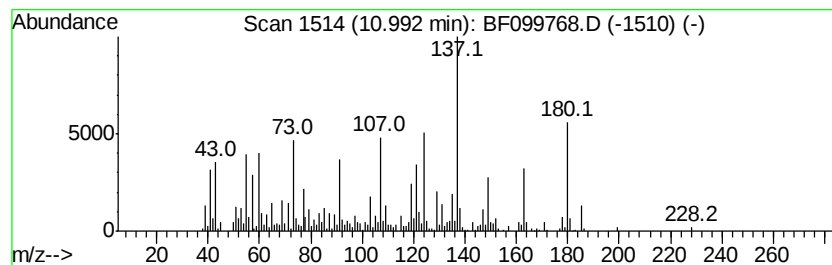
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 4-((1E)-3-Hydroxy-1-propeny... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.99	11.94 ng	619423	Phenanthrene-d10	11.33

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-((1E)-3-Hydroxy-1-propenyl)-2-methoxyphenol	180	C10H12O3	1000297-95-5	95
2			3,7-Benzofurandiol, 2,3-dihydro-	180	C10H12O3	017781-15-6	42
3			(+)-2-Phenethanamine, 1-methyl-	271	C17H21NO2	1000127-89-8	22
4			1-(Prop-2-enyl)-3,4-methylene-	178	C10H10O3	019202-22-3	22
5			(4-Methylphenylthio)acetone	180	C10H12OS	001200-13-1	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102317\
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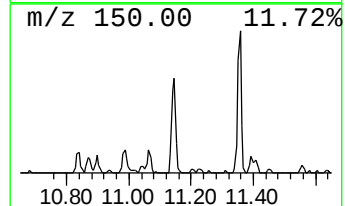
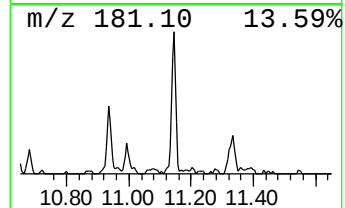
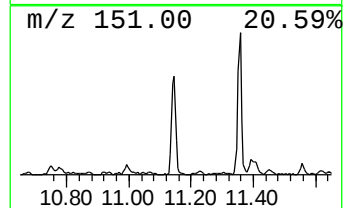
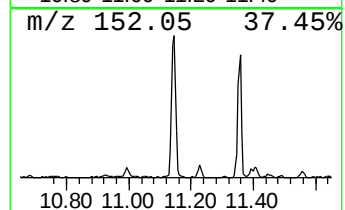
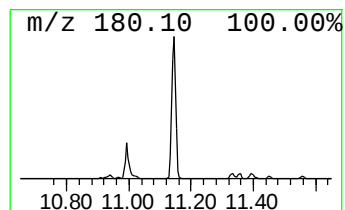
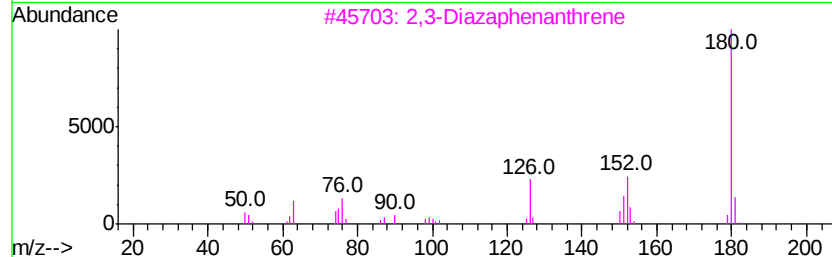
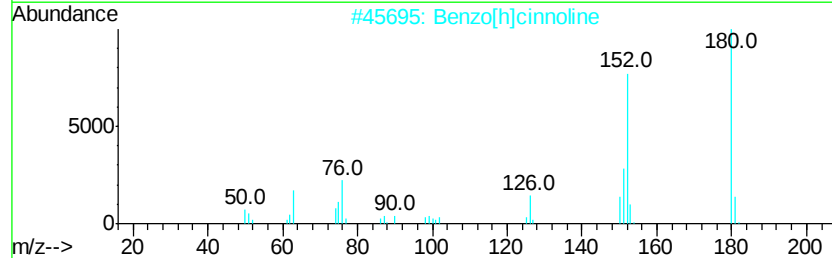
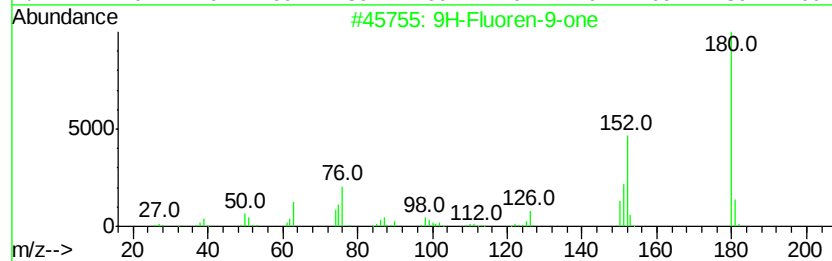
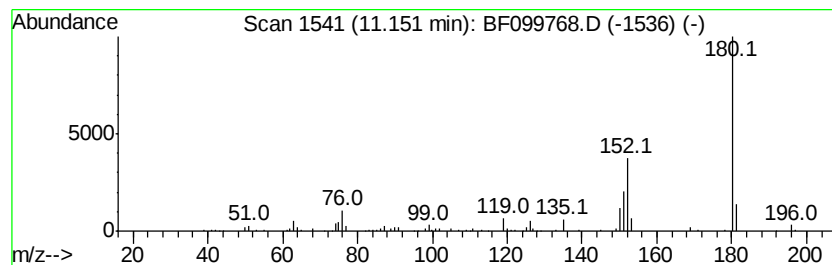
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 9H-Fluoren-9-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.15	5.36 ng	278389	Phenanthrene-d10		11.33	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9H-Fluoren-9-one	180	C13H8O	000486-25-9	96
2		Benzo[h]cinnoline	180	C12H8N2	000230-31-9	91
3		2,3-Diazaphenanthrene	180	C12H8N2	000229-72-1	58
4		1H-Phenalen-1-one	180	C13H8O	000548-39-0	50
5		Thieno[3,2-c]pyridine, 3-nitro-	180	C7H4N2O2S	028783-05-3	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102317\
Data File : BF099768.D
Acq On : 23 Oct 2017 19:30
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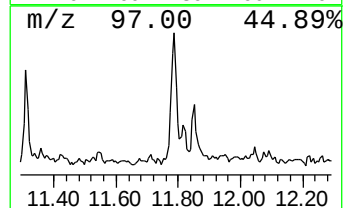
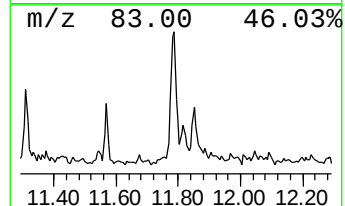
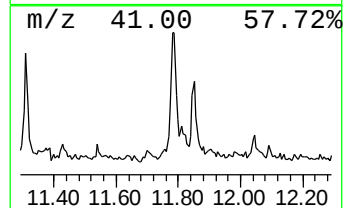
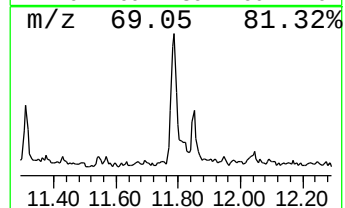
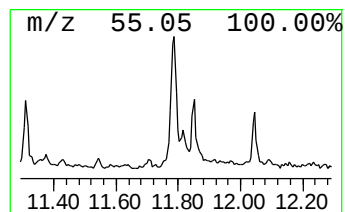
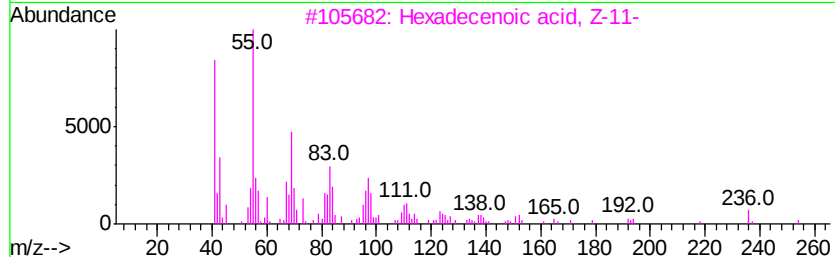
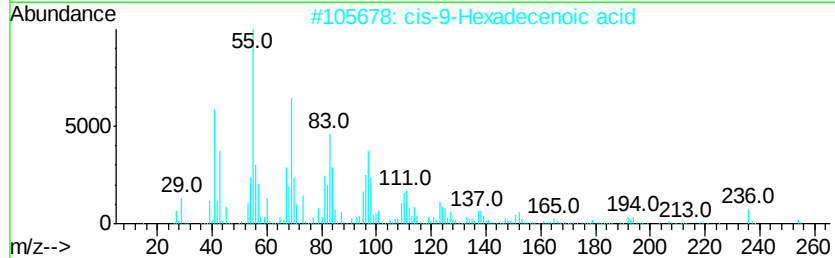
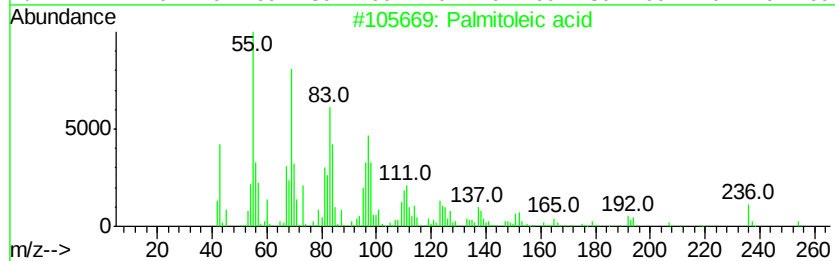
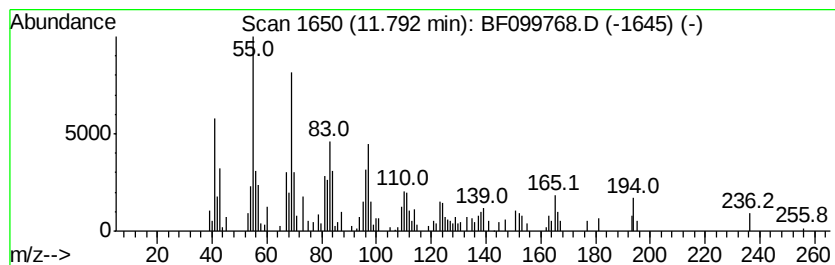
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Palmitoleic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	3.68 ng	190843	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Palmitoleic acid	254	C16H30O2	000373-49-9	94
2		cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	91
3		Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	58
4		E-9-Tetradecenoic acid	226	C14H26O2	1000131-35-8	52
5		3-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-8	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102317\
Data File : BF099768.D
Acq On : 23 Oct 2017 19:30
Operator : SJ/JU
Sample : I5950-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20170723-C-A-COMP2

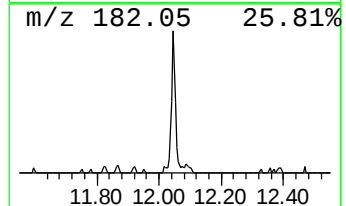
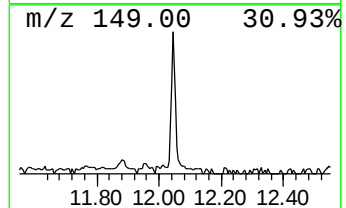
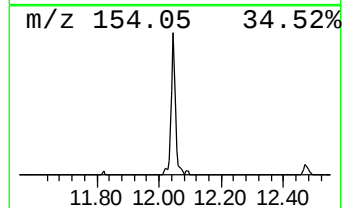
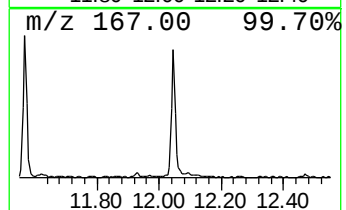
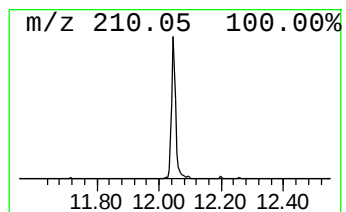
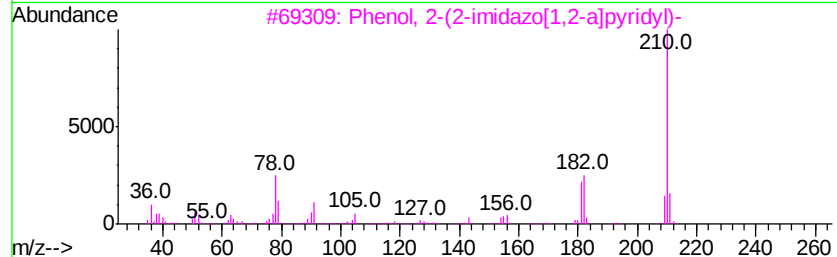
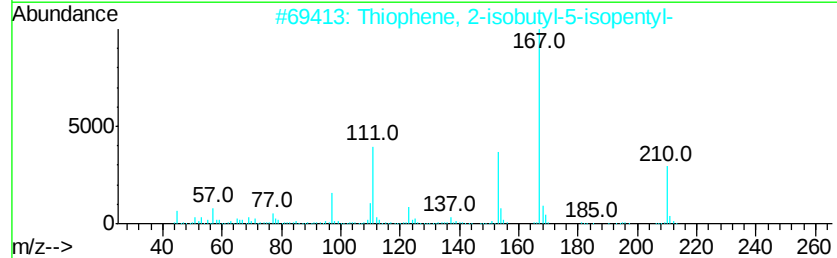
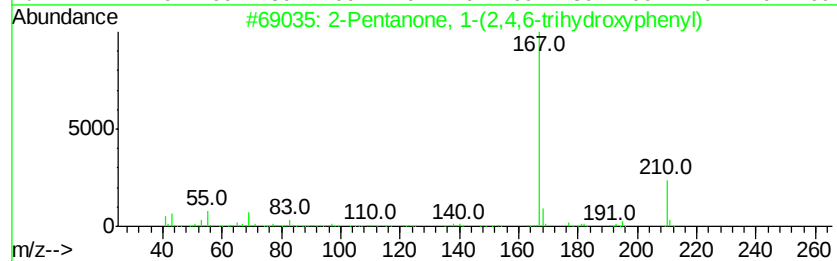
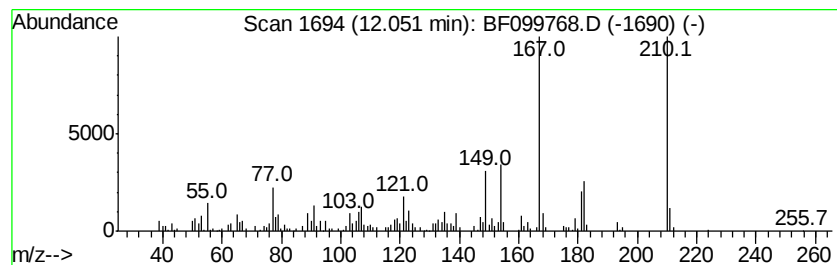
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 2-Pentanone, 1-(2,4,6-trihydroxyphenyl) Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	5.75 ng	298240	Phenanthrene-d10	11.33

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 1-(2,4,6-trihydroxyphenyl)	210	C11H14O4	1000116-22-3	52
2			Thiophene, 2-isobutyl-5-isopentyl-	210	C13H22S	004806-10-4	50
3			Phenol, 2-(2-imidazo[1,2-a]pyridyl)-	210	C13H10N2O	057636-32-5	46
4			1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	41
5			Caffeine, 6-thio-	210	C8H10N4OS	013182-58-6	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102317\
 Data File : BF099768.D
 Acq On : 23 Oct 2017 19:30
 Operator : SJ/JU
 Sample : I5950-10
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20170723-C-A-COMP2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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
Pentanal	2.38	5.6 ng		161534	1	6.80	573005	20.0
1-Pentanol	3.89	15.9 ng		456435	1	6.80	573005	20.0
Hexanal	4.45	25.8 ng		738655	1	6.80	573005	20.0
2-Pentanone, 4-hy...	5.02	5.1 ng		146079	1	6.80	573005	20.0
2-Heptanone	5.60	5.8 ng		166458	1	6.80	573005	20.0
2(5H)-Furanone, 5...	6.21	4.0 ng		114339	1	6.80	573005	20.0
unknown6.57	6.57	71.0 ng		2034480	1	6.80	573005	20.0
1-Hexanol, 2-ethyl-	6.86	3.7 ng		105096	1	6.80	573005	20.0
Heptanoic acid	7.23	17.9 ng		512828	1	6.80	573005	20.0
Hexanoic acid	9.01	3.5 ng		156800	3	9.84	909094	20.0
Vanillin	9.32	4.1 ng		185409	3	9.84	909094	20.0
unknown9.35	9.35	4.9 ng		220867	3	9.84	909094	20.0
Naphthalene, 2,3-...	9.50	3.9 ng		175090	3	9.84	909094	20.0
unknown9.65	9.65	4.2 ng		190625	3	9.84	909094	20.0
unknown10.84	10.84	5.2 ng		268267	4	11.33	1037840	20.0
4-((1E)-3-Hydroxy...	10.99	11.9 ng		619423	4	11.33	1037840	20.0
9H-Fluoren-9-one	11.15	5.4 ng		278389	4	11.33	1037840	20.0
Palmitoleic acid	11.79	3.7 ng		190843	4	11.33	1037840	20.0
2-Pentanone, 1-(2...	12.05	5.8 ng		298240	4	11.33	1037840	20.0