LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126183.D
Acq On : 13 Nov 2021 23:07
Operator : JU/CG
Sample : M4573-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MBR2

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_F\METHODS\8270-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126183.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	13	rVB	6050438	7850531	80.06%	12.286%
2	5.045	499	503	516	rBV2	55793	107650	1.10%	0.168%
3	5.445	567	571	574	rBV	3321655	2950908	30.09%	4.618%
4	6.451	738	742	756	rVB	2836450	2745202	27.99%	4.296%
5	6.828	803	806	810	rBV	1932855	1589305	16.21%	2.487%
6	7.392	896	902	905	rBV	5016356	5361355	54.67%	8.391%
7	8.016	1005	1008	1020	rBV	1021568	1065739	10.87%	1.668%
8	8.116	1020	1025	1028	rBV	2183809	2081720	21.23%	3.258%
9	9.192	1202	1208	1211	rBV	10416912	9806187	100.00%	15.347%
10	9.310	1224	1228	1232	rBV	235961	206845	2.11%	0.324%
11	9.869	1318	1323	1326	rBV	3083620	2526818	25.77%	3.955%
12	10.251	1384	1388	1391	rBV	286575	240726	2.45%	0.377%
13	10.657	1452	1457	1460	rBV	6350264	5646619	57.58%	8.837%
14	10.827	1481	1486	1490	rBV	145637	132544	1.35%	0.207%
15	11.027	1512	1520	1523	rBV	3312383	3001620	30.61%	4.698%
16	11.086	1527	1530	1536	rVB	336558	296037	3.02%	0.463%
17	11.139	1536	1539	1545	rBV	338910	306264	3.12%	0.479%
18	11.351	1570	1575	1579	rBV	2423044	2398647	24.46%	3.754%
19	11.774	1639	1647	1650	rBV	3504829	4132689	42.14%	6.468%
20	11.868	1660	1663	1666	rBV	242605	207165	2.11%	0.324%
21	11.939	1672	1675	1677	rBV	164978	162191	1.65%	0.254%
22	12.145	1707	1710	1713	rVB	1116701	918134	9.36%	1.437%
23	12.215	1719	1722	1724	rBV	154406	136095	1.39%	0.213%
24	12.245	1724	1727	1730	rVB	524665	427768	4.36%	0.669%
25	12.945	1841	1846	1849	rBV	6457433	5884533	60.01%	9.209%
26	13.174	1880	1885	1890	rBV3	67506	102513	1.05%	0.160%
27	13.868	1998	2003	2010	rBV4	49624	104862	1.07%	0.164%
28	13.992	2020	2024	2028	rBV	1582380	1339903	13.66%	2.097%
29	15.456	2268	2273	2277	rBV	1380920	1684291	17.18%	2.636%
30	15.498	2277	2280	2284	rVB	97660	123960	1.26%	0.194%
31	15.927	2350	2353	2359	rVB	81766	123909	1.26%	0.194%
32	16.433	2435	2439	2446	rVB2	76400	130800	1.33%	0.205%
33	17.021	2534	2539	2548	rVB2	50849	103140	1.05%	0.161%

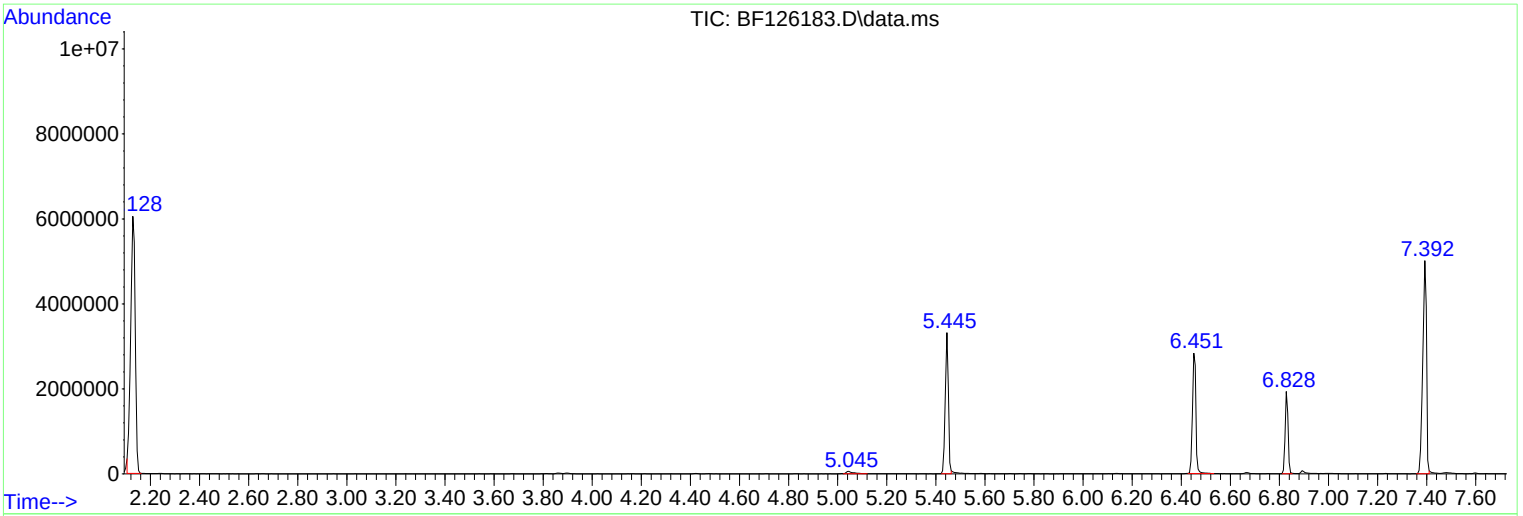
Sum of corrected areas: 63896670

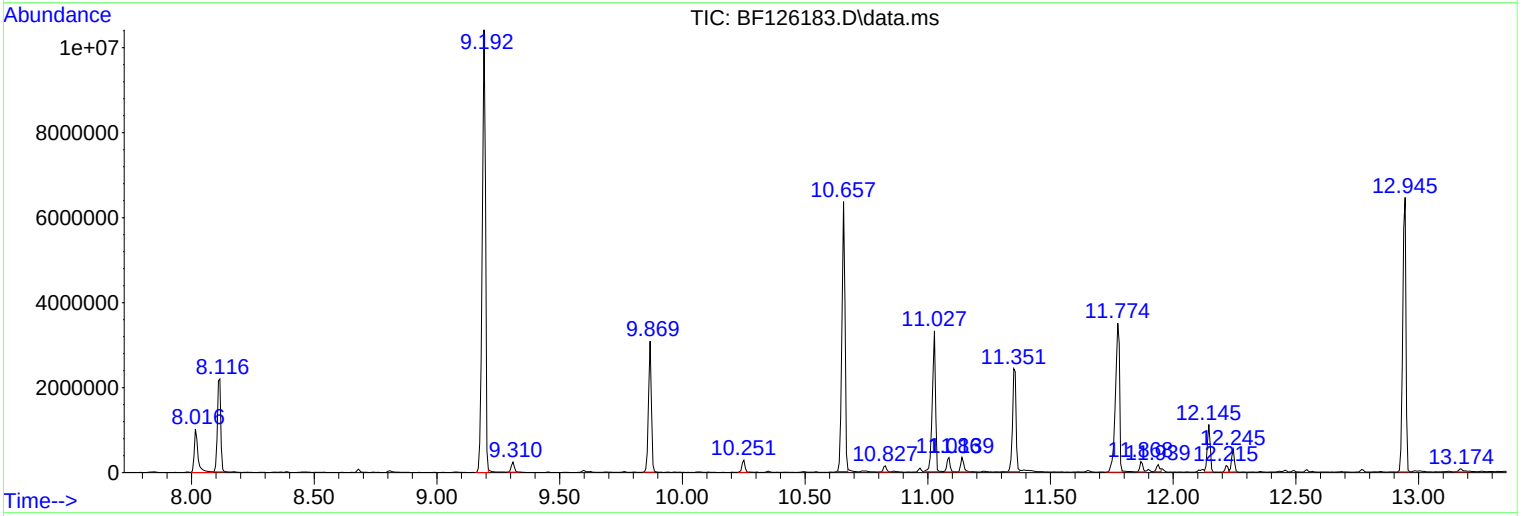
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126183.D
Acq On : 13 Nov 2021 23:07
Operator : JU/CG
Sample : M4573-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

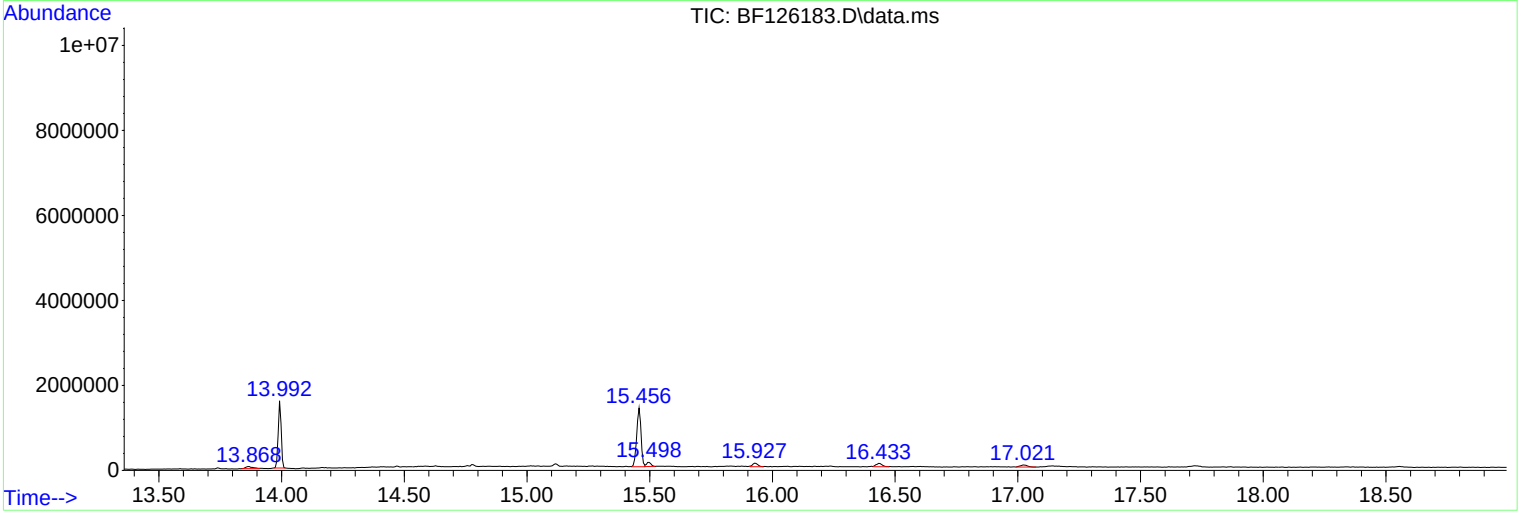
Instrument :
BNA_F
ClientSampleId :
MBR2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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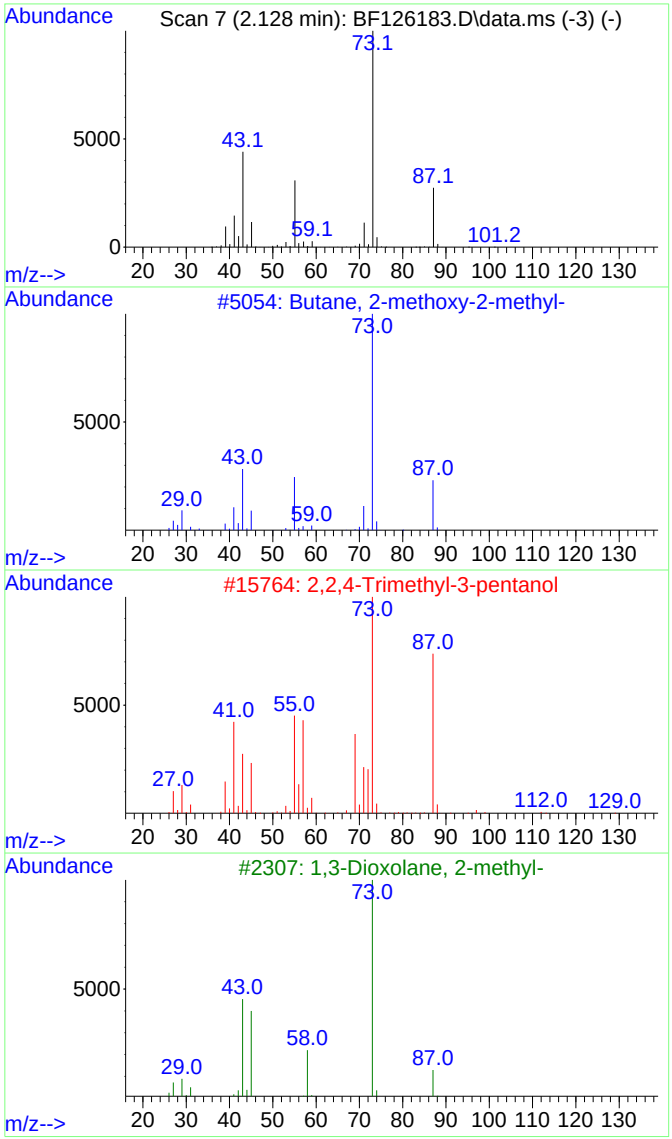
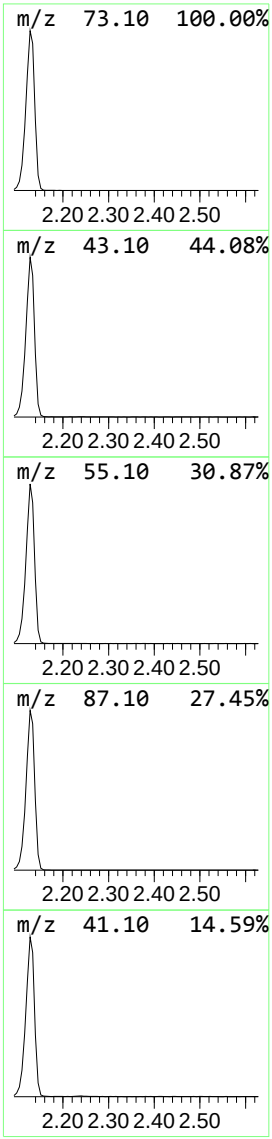
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	98.79 ng	7850530	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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

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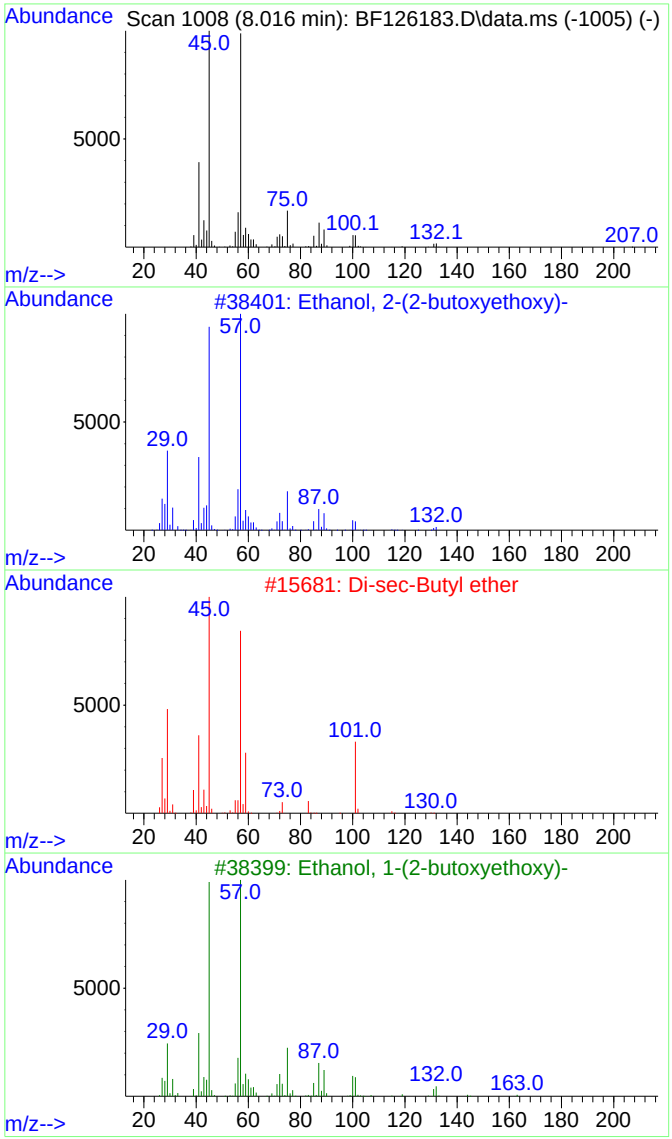
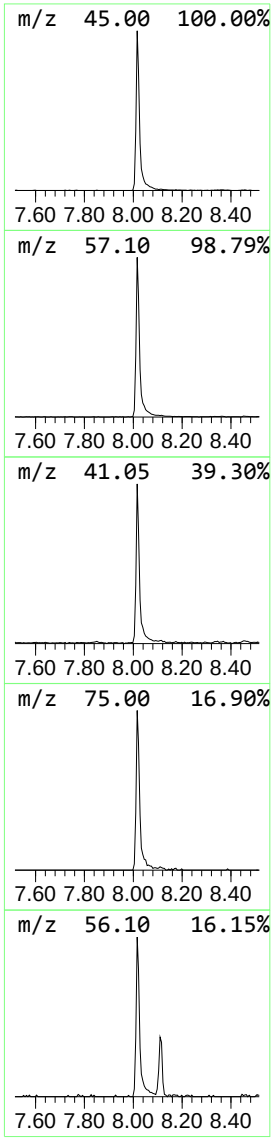
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	10.24 ng	1065740	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
3	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MBR2

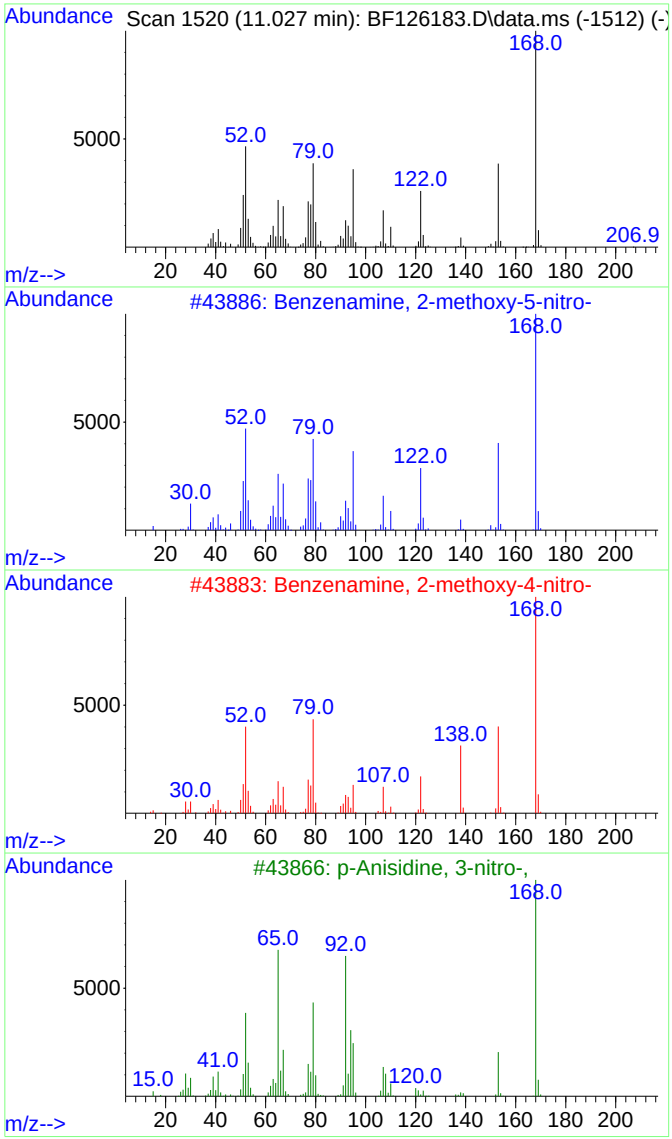
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

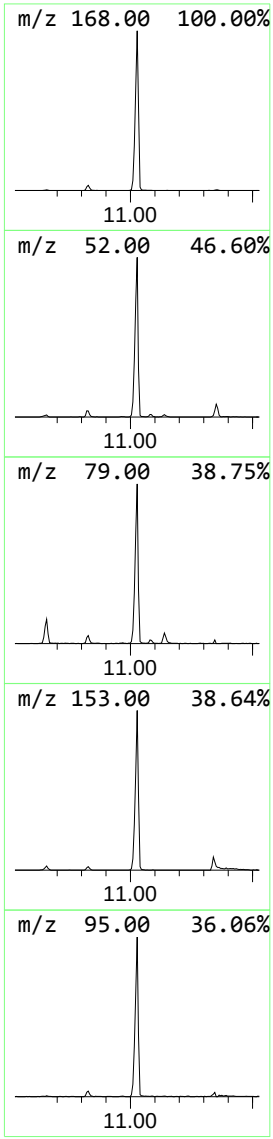
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzenamine, 2-methoxy-5-ni... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.027	25.03 ng	3001620	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2-methoxy-5-nitro-	168	C7H8N2O3	000099-59-2	98
2	Benzenamine, 2-methoxy-4-nitro-	168	C7H8N2O3	000097-52-9	86
3	p-Anisidine, 3-nitro-,	168	C7H8N2O3	000577-72-0	64
4	Benzenamine, 4-methoxy-2-nitro-	168	C7H8N2O3	000096-96-8	64
5	6-Thioxo-1,5,6,7-tetrahydro-4H-p...	168	C5H4N4OS	024521-76-4	47





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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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TIC Library : C:\Database\NIST20.L
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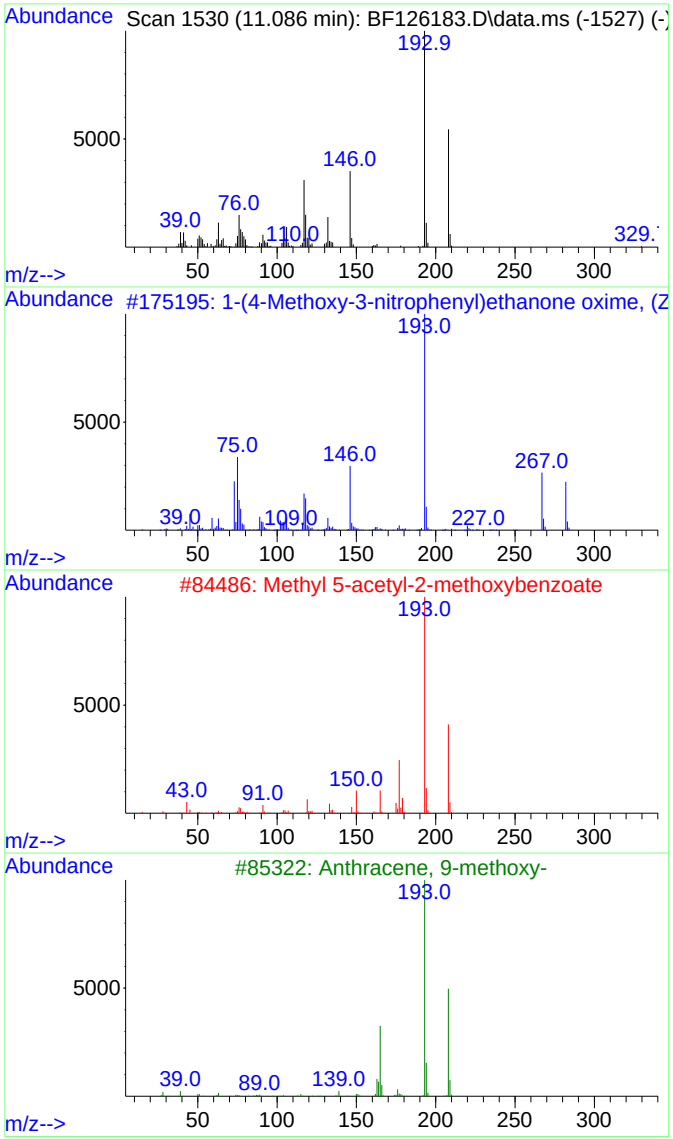
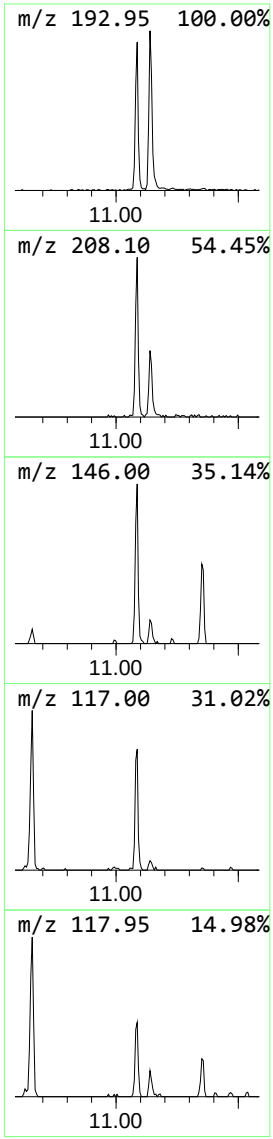
****
Peak Number 4 1-(4-Methoxy-3-nitrophenyl)... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.086	2.47 ng	296037	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Methoxy-3-nitrophenyl)ethan...	282	C12H18N2O4Si	1000373-42-2	53
2	Methyl 5-acetyl-2-methoxybenzoate	208	C11H12O4	039971-36-3	49
3	Anthracene, 9-methoxy-	208	C15H12O	002395-96-2	47
4	1H-Pyrazole, 3,5-bis(1,1-dimethy...	208	C13H24N2	125281-21-2	47
5	1,2,5,6-Tetramethylacenaphthylene	208	C16H16	132118-73-1	38





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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TIC Library : C:\Database\NIST20.L
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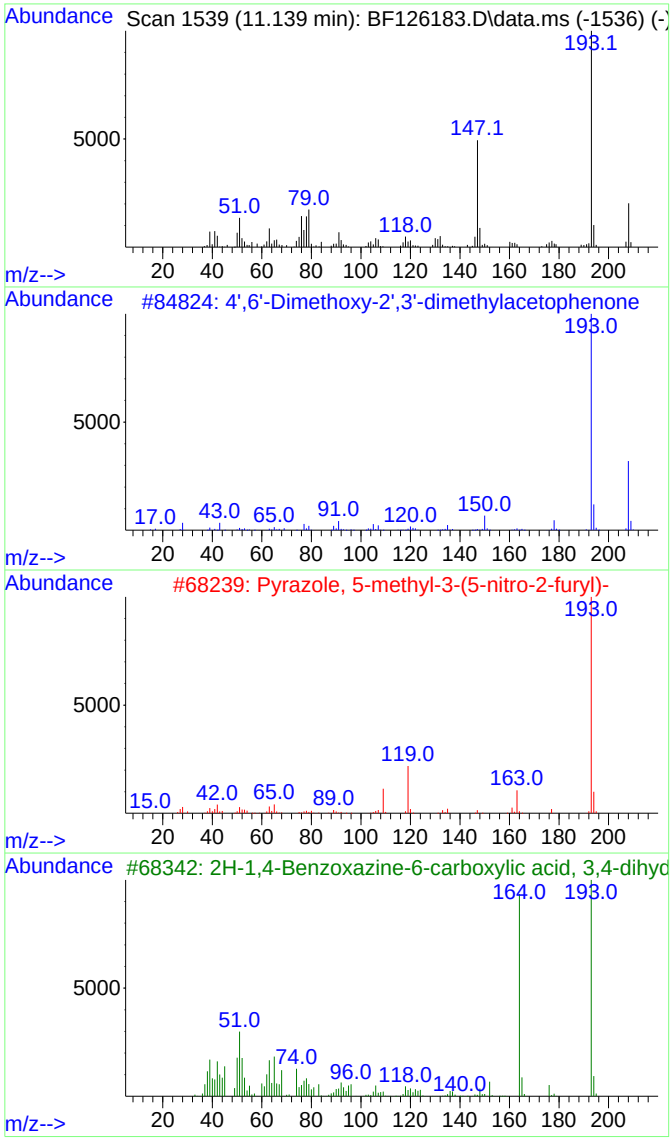
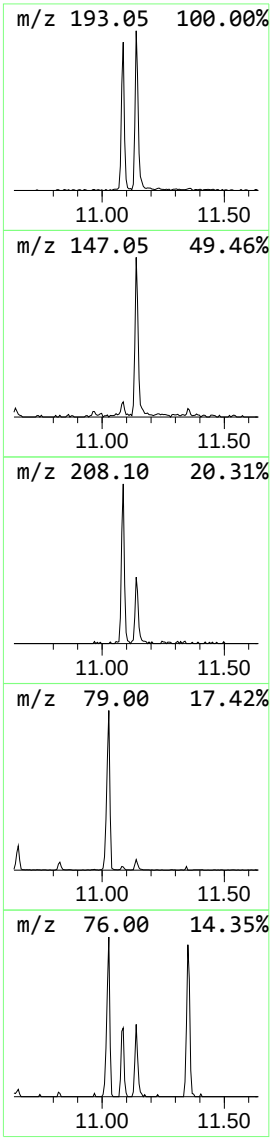
****

Peak Number 5 unknown11.139 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.139	2.55 ng	306264	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4',6'-Dimethoxy-2',3'-dimethylac...	208	C12H16O3	1010244-80-3	47
2	Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	43
3	2H-1,4-Benzoxazine-6-carboxylic ...	193	C9H7NO4	1000351-35-0	43
4	Benzaldehyde, p-nitro-, dimethyl...	193	C9H11N3O2	010424-92-7	43
5	benzenamine, 3,5-dimethyl-N-(1-m...	208	C11H16N2O2	1000400-57-7	41





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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
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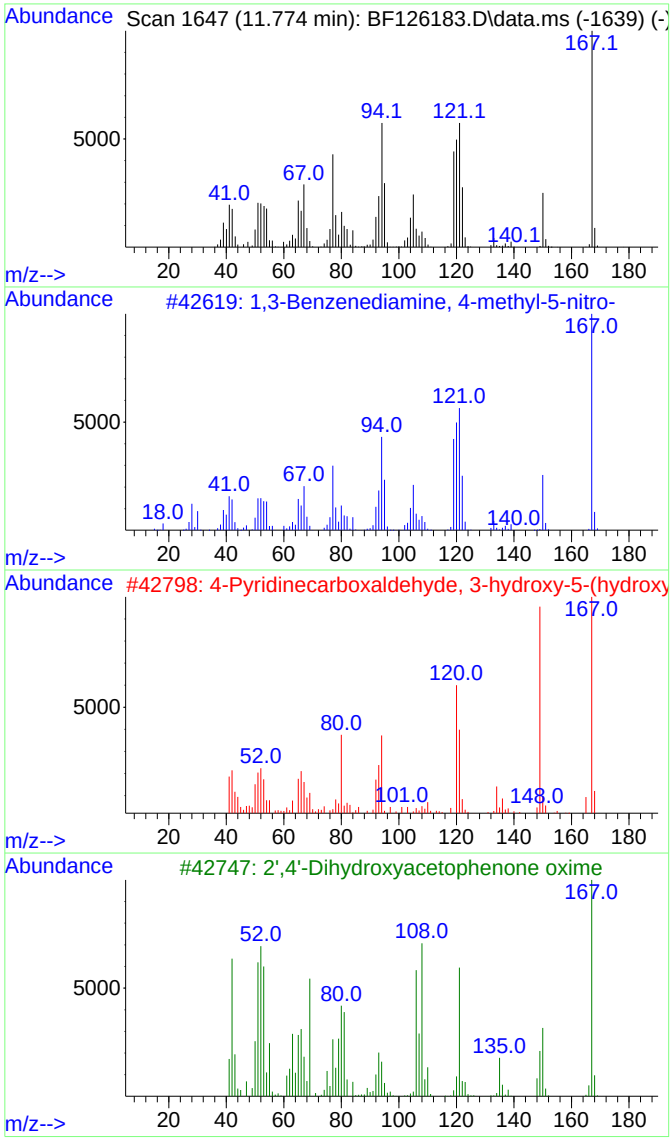
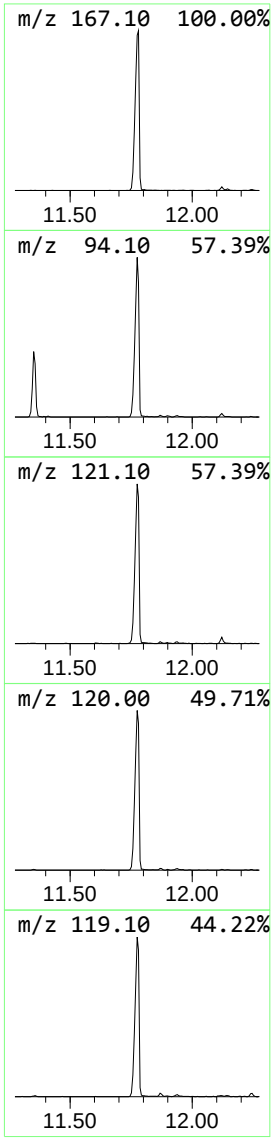
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Benzenediamine, 4-methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.774	34.46 ng	4132690	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenediamine, 4-methyl-5-n...	167	C7H9N3O2	006629-29-4	99
2	4-Pyridinecarboxaldehyde, 3-hydr...	167	C8H9NO3	000066-72-8	49
3	2',4'-Dihydroxyacetophenone oxime	167	C8H9NO3	1000212-89-5	38
4	3,5-Pyridinedicarboxylic acid	167	C7H5NO4	000499-81-0	25
5	2-Methylamino-5-nitroaniline (is...	167	C7H9N3O2	1000477-10-5	25





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TIC Library : C:\Database\NIST20.L
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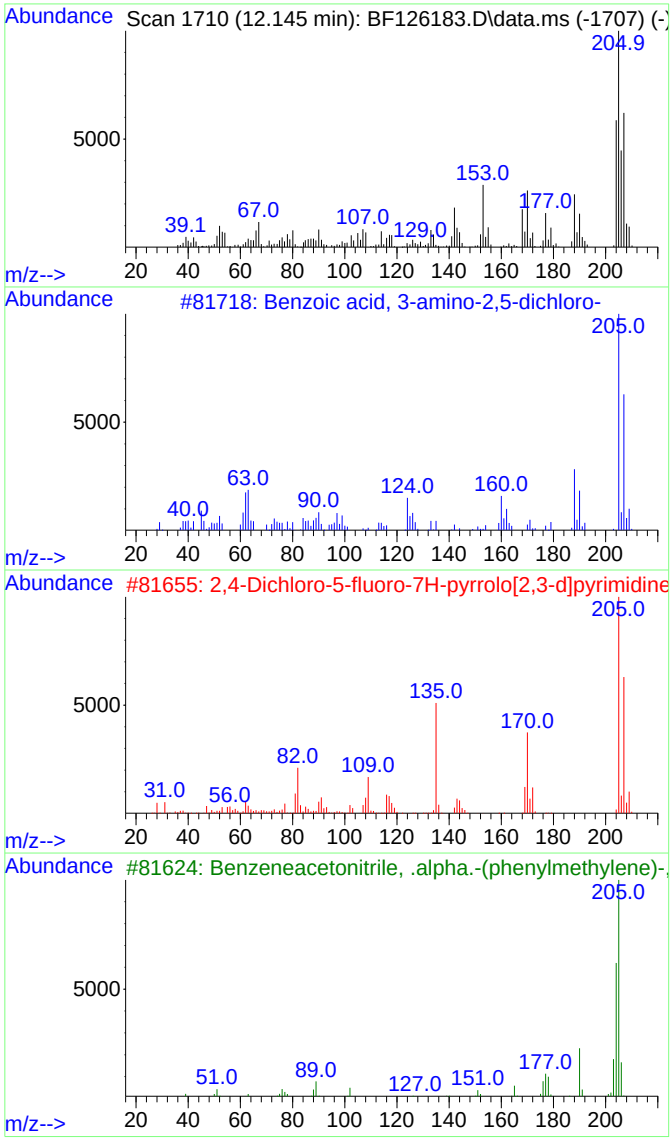
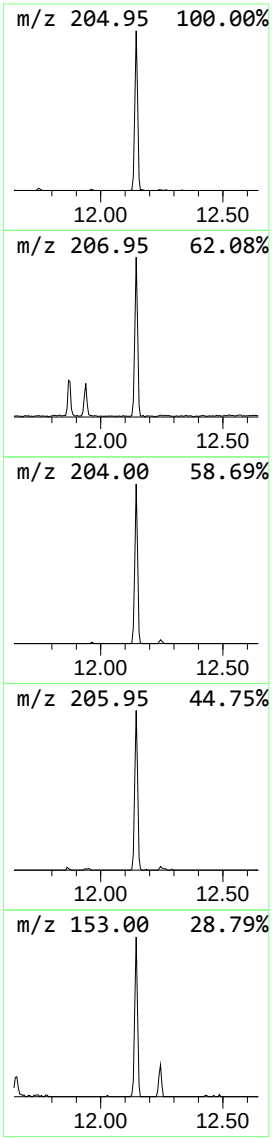
****
Peak Number 7 Benzoic acid, 3-amino-2,5-d... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.145	7.66 ng	918134	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	60
2	2,4-Dichloro-5-fluoro-7H-pyrrolo...	205	C6H2Cl2FN3	1053228-29-7	38
3	Benzeneacetonitrile, .alpha.-(ph...	205	C15H11N	016610-80-3	38
4	Benzonitrile, 4-(2-phenylethenyl...	205	C15H11N	013041-79-7	38
5	Quinoline, 2-phenyl-	205	C15H11N	000612-96-4	35





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TIC Library : C:\Database\NIST20.L
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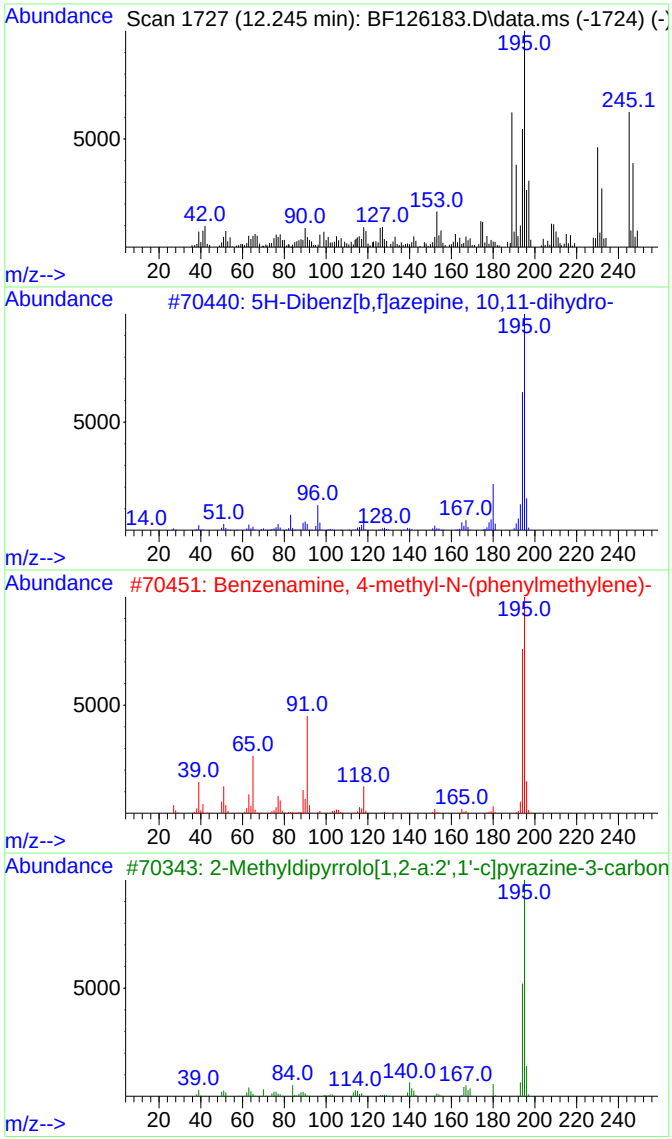
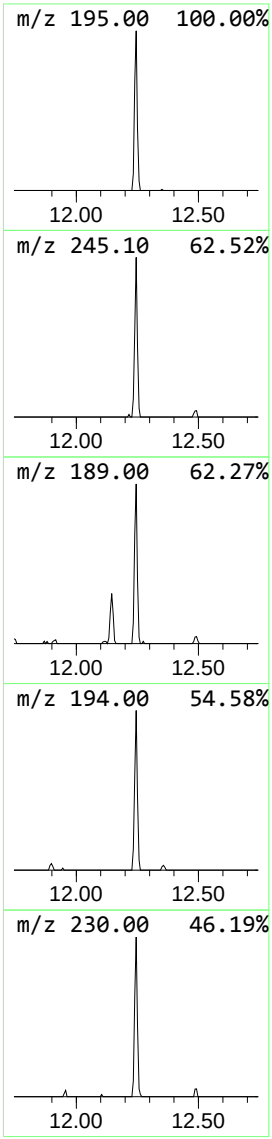
****

Peak Number 8 unknown12.245 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.245	3.57 ng	427768	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Dibenz[b,f]azepine, 10,11-dih...	195	C14H13N	000494-19-9	25
2	Benzenamine, 4-methyl-N-(phenylm...	195	C14H13N	002272-45-9	25
3	2-Methyldipyrrolo[1,2-a:2',1'-c]...	195	C12H9N3	1010305-64-5	22
4	3,4,5-Trimethoxybenzoyl chloride	230	C10H11ClO4	004521-61-3	22
5	Benzenamine, 4-(2-phenylethenyl)-	195	C14H13N	000834-24-2	18





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.128	98.8	ng	7850530	1	6.828	1589310	20.0
Ethanol, 2-(2-b...	8.016	10.2	ng	1065740	2	8.116	2081720	20.0
Benzenamine, 2-...	11.027	25.0	ng	3001620	4	11.357	2398650	20.0
1-(4-Methoxy-3-...	11.086	2.5	ng	296037	4	11.357	2398650	20.0
unknown11.139	11.139	2.5	ng	306264	4	11.357	2398650	20.0
1,3-Benzenediam...	11.774	34.5	ng	4132690	4	11.357	2398650	20.0
Benzoic acid, 3...	12.145	7.7	ng	918134	4	11.357	2398650	20.0
unknown12.245	12.245	3.6	ng	427768	4	11.357	2398650	20.0