

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
 Data File : BF124781.D
 Acq On : 27 Jul 2021 00:20
 Operator : JU/CG
 Sample : M3118-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20210546-COM-19

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-BF072221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124781.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	8	11	15	rBB2	10001	11121	11.70%	1.536%
2	5.093	508	511	513	rBB	1524	1454	1.53%	0.201%
3	5.487	574	578	581	rBB	104258	95057	100.00%	13.127%
4	6.498	745	750	753	rBV	103344	94221	99.12%	13.012%
5	6.875	811	814	817	rBB	37958	28731	30.23%	3.968%
6	7.434	905	909	912	rBB	73163	57940	60.95%	8.002%
7	8.051	1012	1014	1020	rBB	23126	19084	20.08%	2.635%
8	8.157	1028	1032	1035	rBB	50501	37649	39.61%	5.199%
9	9.228	1211	1214	1217	rBV	118737	89813	94.48%	12.403%
10	9.910	1327	1330	1333	rBB	47282	35696	37.55%	4.930%
11	10.698	1461	1464	1467	rBB	60497	45121	47.47%	6.231%
12	11.398	1580	1583	1586	rBV	42864	31560	33.20%	4.358%
13	12.610	1787	1789	1792	rBB	4511	2912	3.06%	0.402%
14	12.839	1825	1828	1831	rBB	6982	5349	5.63%	0.739%
15	12.980	1849	1852	1855	rBV	92990	74585	78.46%	10.300%
16	13.886	2003	2006	2007	rBV	1693	1762	1.85%	0.243%
17	13.898	2007	2008	2013	rVB2	2630	2105	2.21%	0.291%
18	14.039	2028	2032	2035	rBV	34860	30901	32.51%	4.267%
19	14.063	2035	2036	2039	rVB	2170	1234	1.30%	0.170%
20	14.198	2056	2059	2061	rBV	2350	2106	2.22%	0.291%
21	14.327	2078	2081	2084	rBB	1370	1222	1.29%	0.169%
22	14.457	2100	2103	2106	rBV	1016	1202	1.26%	0.166%
23	14.504	2106	2111	2114	rVV	1928	2278	2.40%	0.315%
24	14.810	2159	2163	2166	rBV	1868	2704	2.84%	0.373%
25	15.074	2203	2208	2209	rBV2	2407	2155	2.27%	0.298%
26	15.104	2212	2213	2218	rVB3	1024	1153	1.21%	0.159%
27	15.151	2218	2221	2224	rVB2	1642	2102	2.21%	0.290%
28	15.204	2227	2230	2233	rBV	1630	2023	2.13%	0.279%
29	15.392	2258	2262	2265	rVB3	2096	2590	2.72%	0.358%
30	15.451	2269	2272	2273	rBV2	1650	1440	1.51%	0.199%
31	15.515	2279	2283	2288	rBV	19501	23071	24.27%	3.186%
32	15.633	2301	2303	2307	rVB	1151	1462	1.54%	0.202%
33	15.668	2307	2309	2311	rBV	1552	1442	1.52%	0.199%
34	15.774	2325	2327	2330	rVB2	1354	1139	1.20%	0.157%
35	15.974	2357	2361	2364	rBV3	1195	1441	1.52%	0.199%
36	16.104	2379	2383	2385	rBV2	1402	1471	1.55%	0.203%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.492	2444	2449	2450	rBV	1022	1350	1.42%	0.186%
38	16.757	2490	2494	2496	rBV	1046	1573	1.65%	0.217%
39	17.627	2640	2642	2645	rBV	806	1311	1.38%	0.181%
40	17.892	2684	2687	2689	rBV	1118	1162	1.22%	0.160%
41	18.603	2805	2808	2812	rVB	1061	1422	1.50%	0.196%

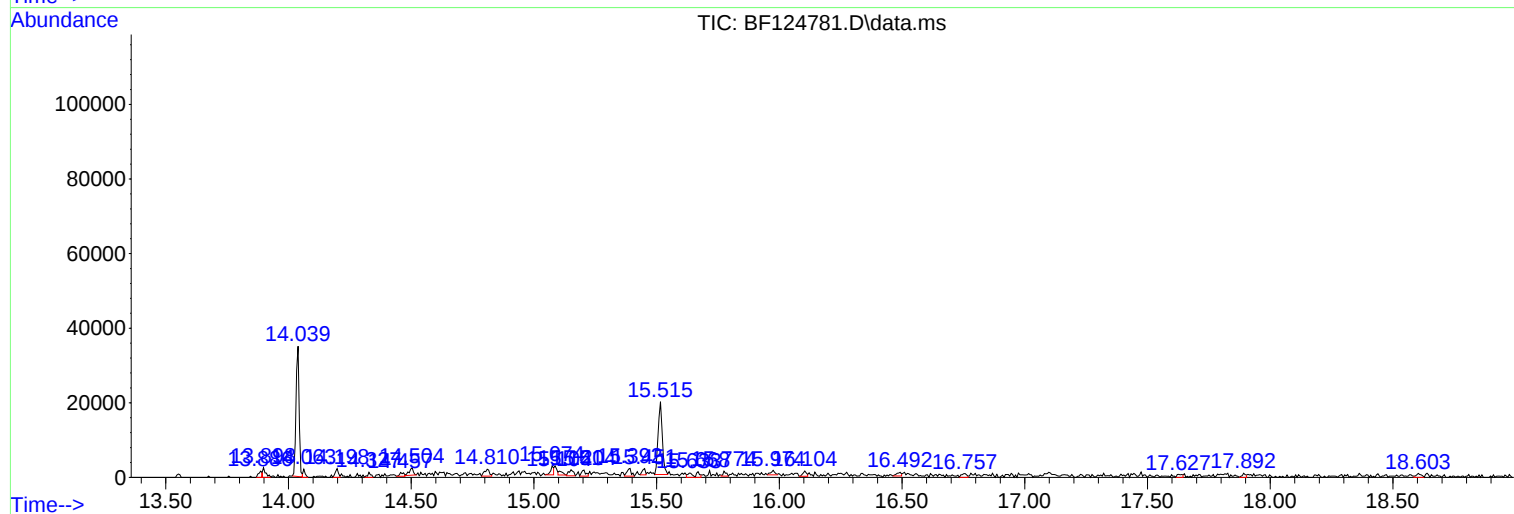
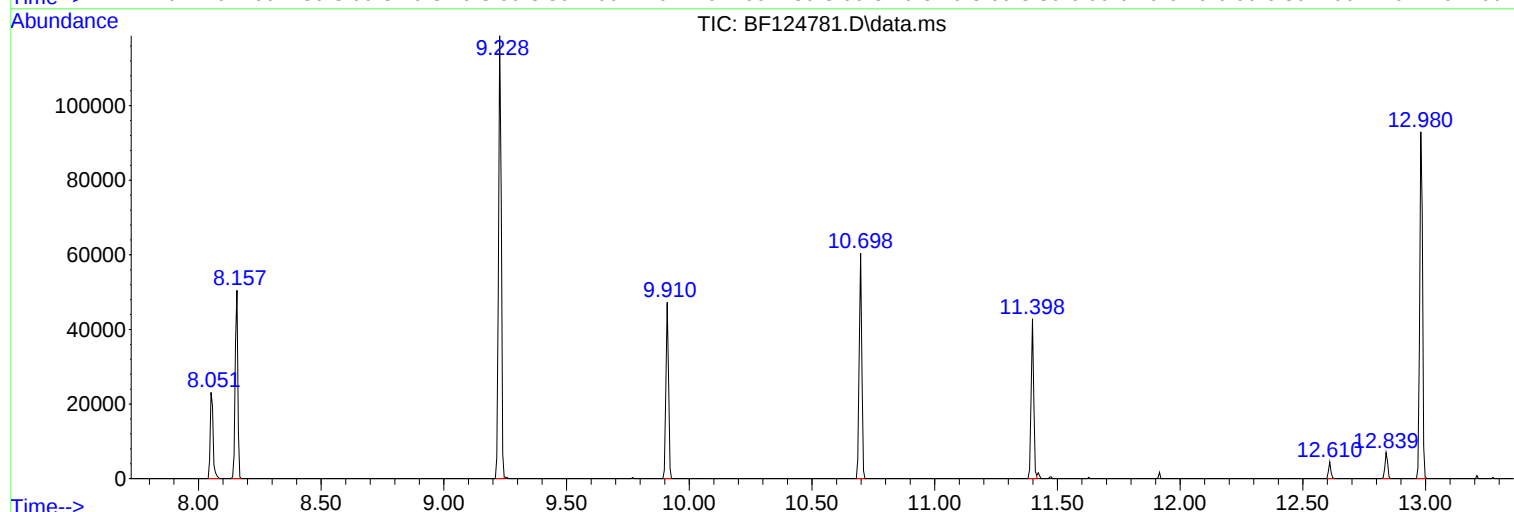
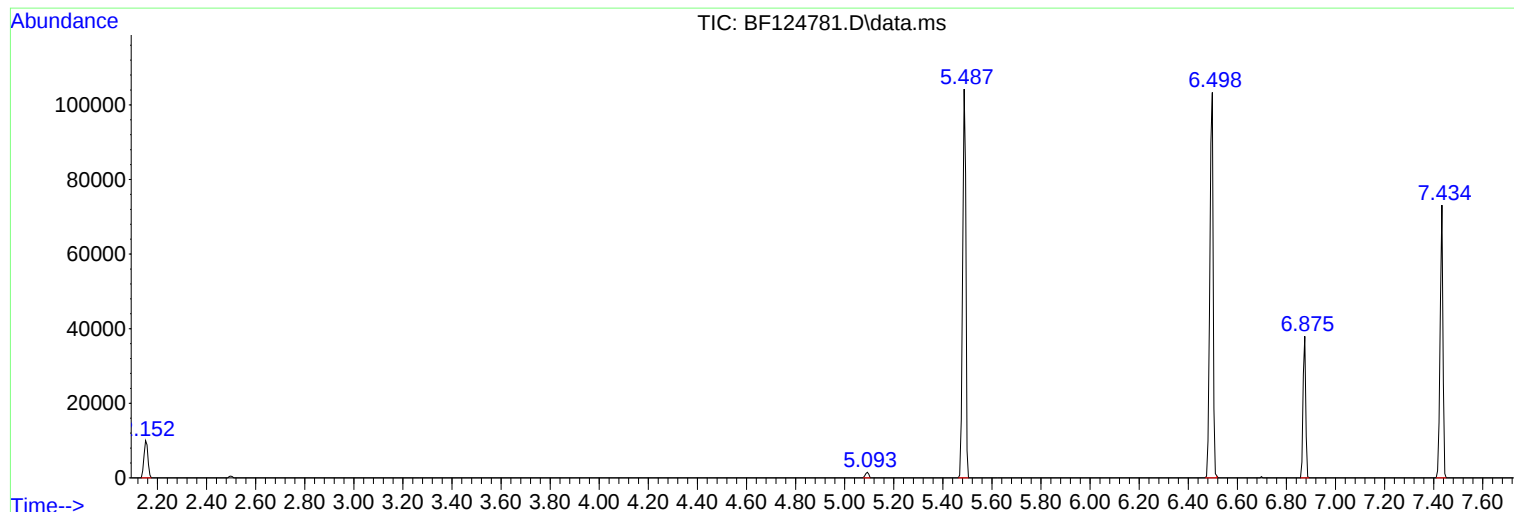
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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20210546-COM-19

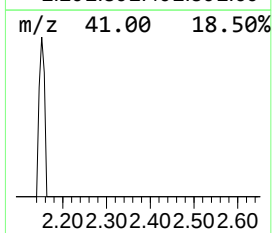
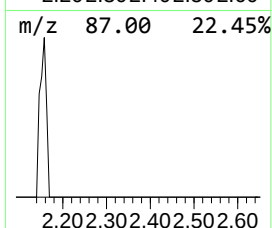
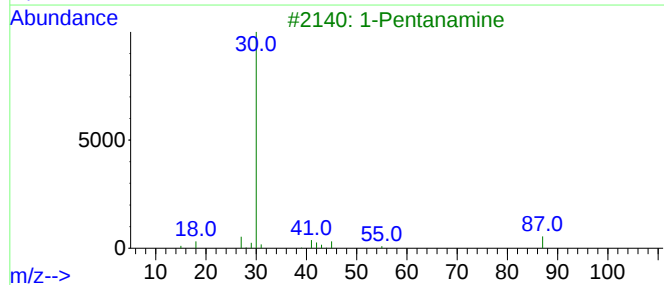
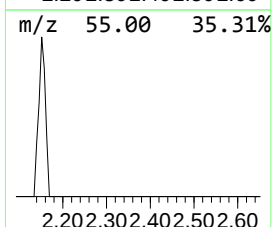
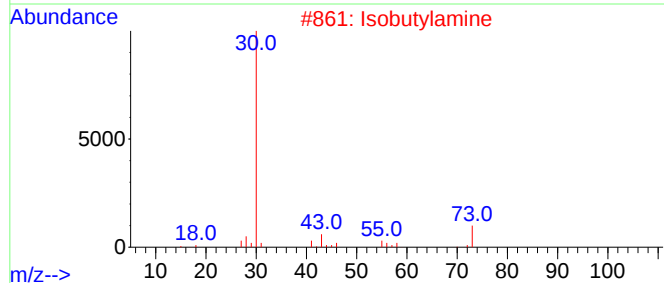
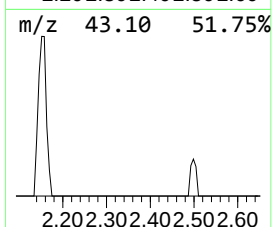
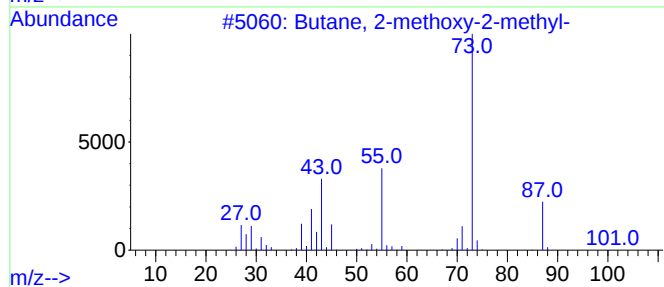
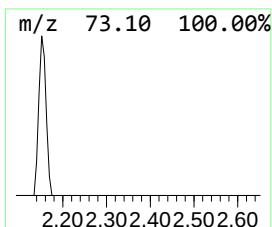
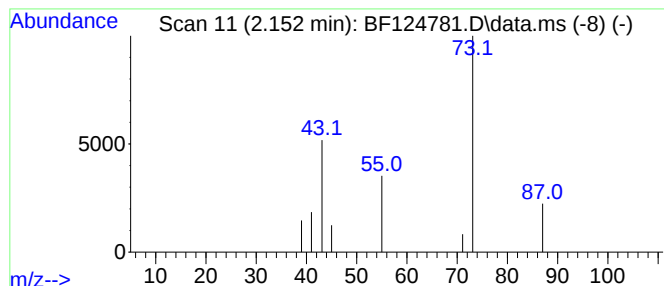
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	7.74 ng	11121	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	3



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ALS Vial : 19 Sample Multiplier: 1

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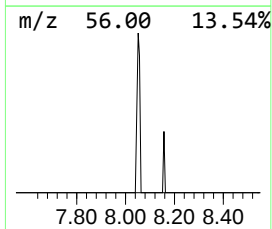
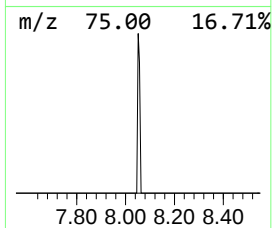
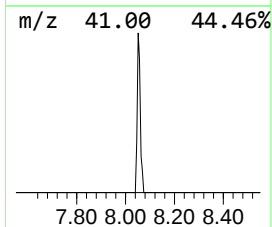
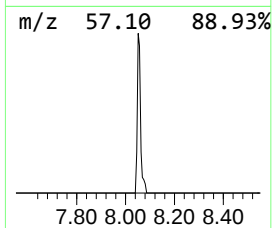
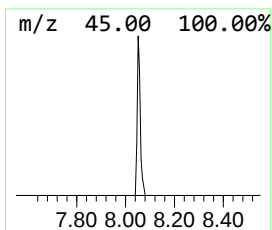
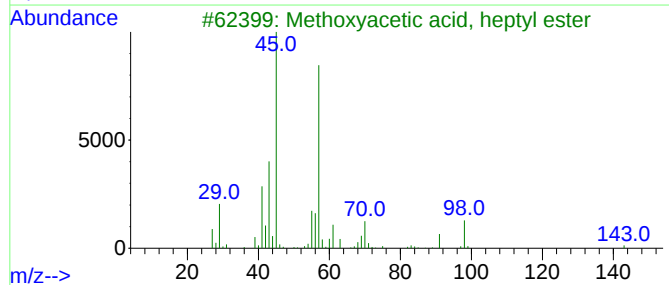
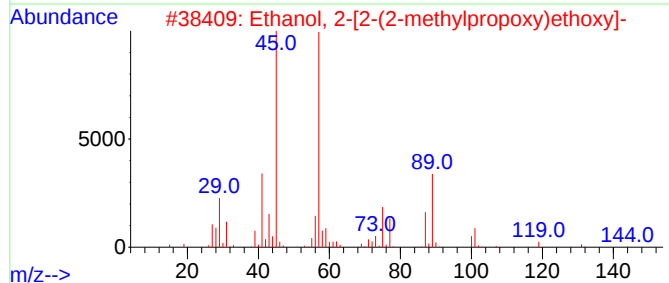
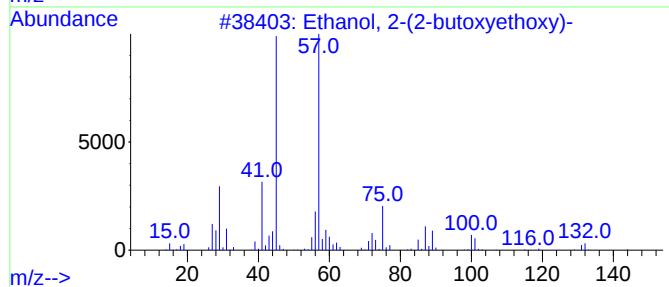
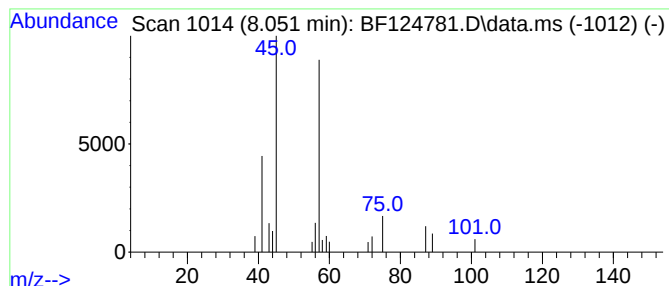
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	10.14 ng	19084	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	45
4			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	39
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	39



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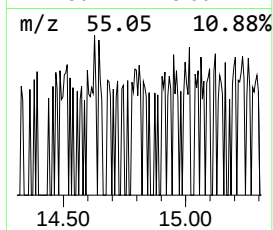
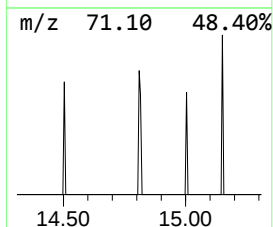
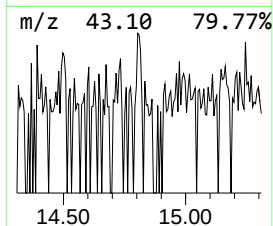
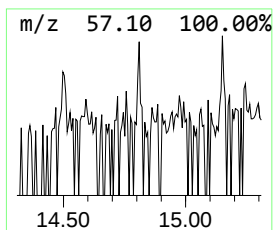
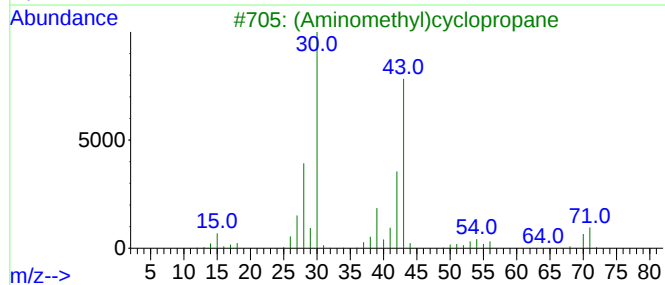
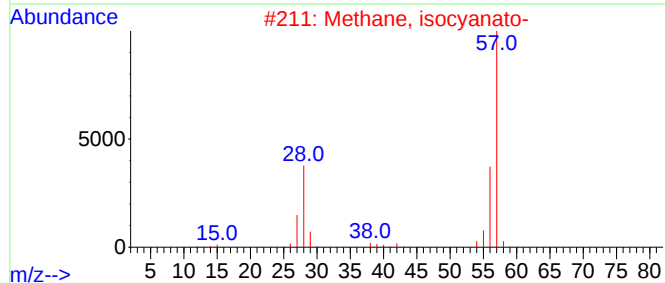
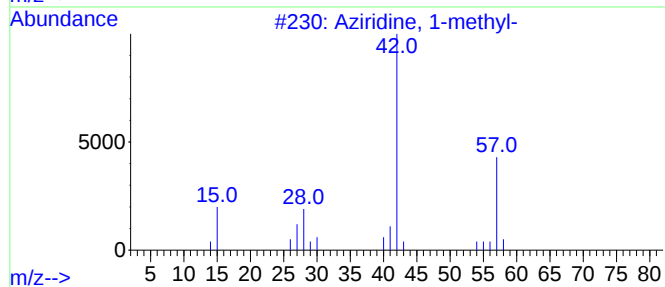
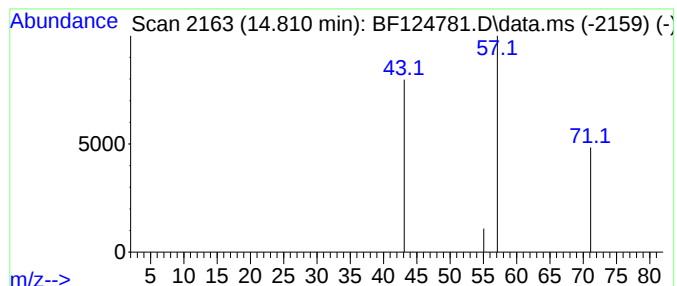
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown14.810 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	2.34 ng	2704	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aziridine, 1-methyl-	57	C3H7N	001072-44-2	3
2			Methane, isocyanato-	57	C2H3NO	000624-83-9	3
3			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
4			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	2
5			Ethanamine, N-methylene-	57	C3H7N	043729-97-1	2



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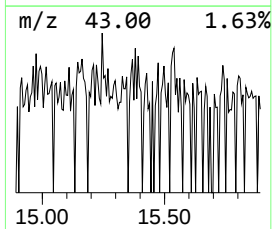
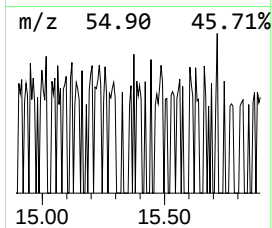
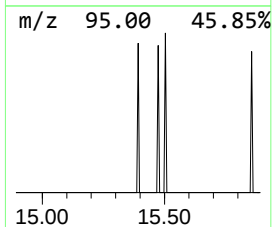
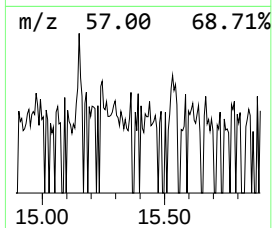
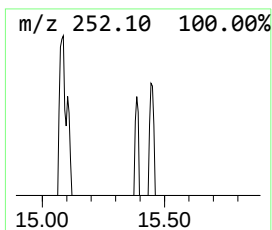
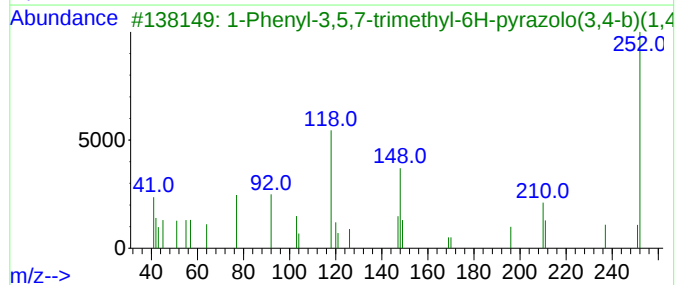
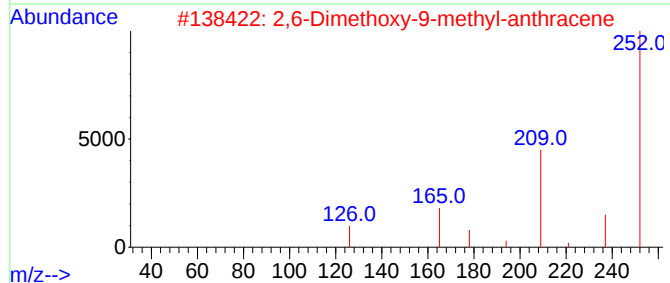
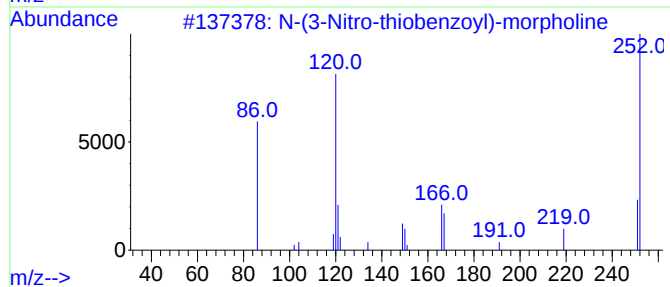
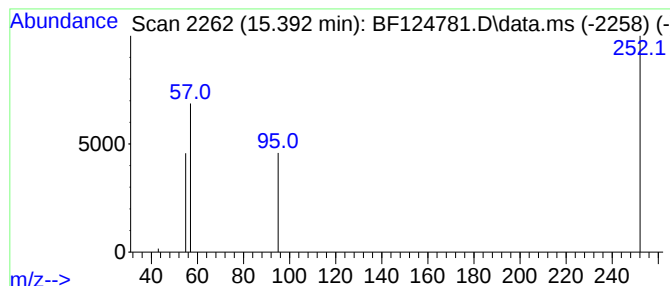
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.392 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	2.25 ng	2590	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(3-Nitro-thiobenzoyl)-morpholine	252	C11H12N2O3S	050903-05-4	3
2			2,6-Dimethoxy-9-methyl-anthracene	252	C17H16O2	110038-59-0	3
3			1-Phenyl-3,5,7-trimethyl-6H-pyra...	252	C15H16N4	063536-14-1	3
4			Propargyl alcohol, heptafluorobu...	252	C7H3F7O2	1000352-28-1	2
5			3,4-Octadiene, 2,2-dimethyl-	138	C10H18	034511-02-9	1



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.152	7.7	ng	11121	1	6.875	28731	20.0
Ethanol, 2-(2-b...	8.051	10.1	ng	19084	2	8.157	37649	20.0
unknown14.810	14.810	2.3	ng	2704	6	15.515	23071	20.0
unknown15.392	15.392	2.3	ng	2590	6	15.515	23071	20.0