

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072321\
 Data File : BF124734.D
 Acq On : 24 Jul 2021 2:46
 Operator : JU/CG
 Sample : M3139-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SEW-RO

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: BF124734.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	12	15	18	rBB	4603	4948	3.74%	0.523%
2	5.087	506	510	514	rBB	11796	12892	9.74%	1.362%
3	5.481	573	577	580	rBB	107420	95247	71.93%	10.061%
4	6.486	744	748	751	rBB	106451	97230	73.43%	10.270%
5	6.869	810	813	816	rBB	48144	36121	27.28%	3.815%
6	7.428	904	908	911	rBB	74841	65544	49.50%	6.923%
7	8.045	1011	1013	1016	rBB	3934	3032	2.29%	0.320%
8	8.151	1027	1031	1034	rBB	65650	52257	39.47%	5.520%
9	9.227	1209	1214	1217	rBB	168239	132408	100.00%	13.986%
10	9.904	1326	1329	1332	rBB	74524	61002	46.07%	6.443%
11	10.333	1400	1402	1404	rBB	3207	2369	1.79%	0.250%
12	10.557	1434	1440	1444	rBV2	2636	4733	3.57%	0.500%
13	10.692	1460	1463	1466	rBV	89547	69531	52.51%	7.344%
14	10.821	1478	1485	1488	rBV2	9106	13947	10.53%	1.473%
15	10.886	1492	1496	1500	rBV5	2580	5001	3.78%	0.528%
16	10.957	1505	1508	1511	rBV3	1859	2440	1.84%	0.258%
17	11.033	1517	1521	1523	rVB4	1640	1682	1.27%	0.178%
18	11.169	1542	1544	1546	rBV2	2262	1806	1.36%	0.191%
19	11.257	1557	1559	1561	rBV3	2709	1873	1.41%	0.198%
20	11.286	1562	1564	1567	rVB2	5220	4187	3.16%	0.442%
21	11.392	1579	1582	1585	rBV	84405	62972	47.56%	6.652%
22	11.686	1630	1632	1635	rVB3	6092	4994	3.77%	0.528%
23	11.845	1657	1659	1661	rVB3	2753	1893	1.43%	0.200%
24	11.868	1661	1663	1668	rBV6	2479	4449	3.36%	0.470%
25	11.916	1668	1671	1673	rVV3	10153	8536	6.45%	0.902%
26	12.374	1746	1749	1753	rVB4	3589	5323	4.02%	0.562%
27	12.580	1782	1784	1786	rBV3	1858	1950	1.47%	0.206%
28	12.698	1801	1804	1808	rBV4	5708	5978	4.51%	0.631%
29	12.751	1811	1813	1817	rVV5	2061	2199	1.66%	0.232%
30	12.798	1819	1821	1825	rVB4	1437	1865	1.41%	0.197%
31	12.974	1848	1851	1855	rVB	118455	108533	81.97%	11.464%
32	13.257	1895	1899	1905	rVB3	1622	2814	2.13%	0.297%
33	13.874	1998	2004	2006	rBV2	3286	5497	4.15%	0.581%
34	13.898	2006	2008	2011	rVB2	3838	3023	2.28%	0.319%
35	14.027	2027	2030	2033	rVB	37606	30832	23.29%	3.257%
36	15.498	2276	2280	2284	rBB	25372	27618	20.86%	2.917%

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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

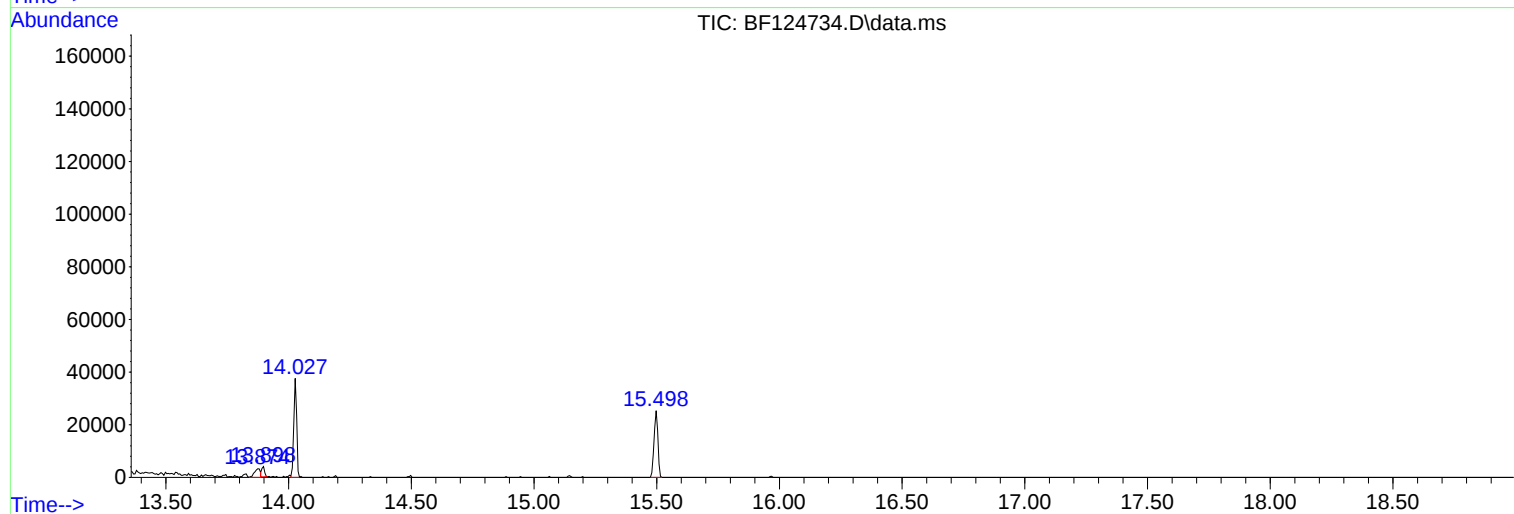
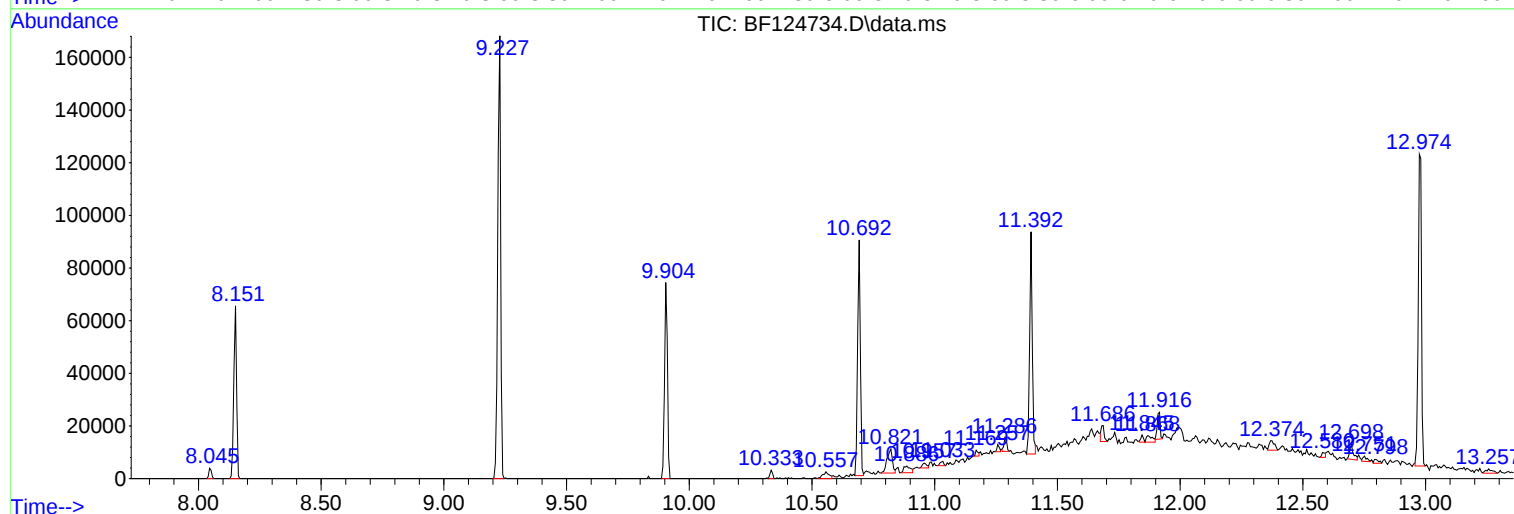
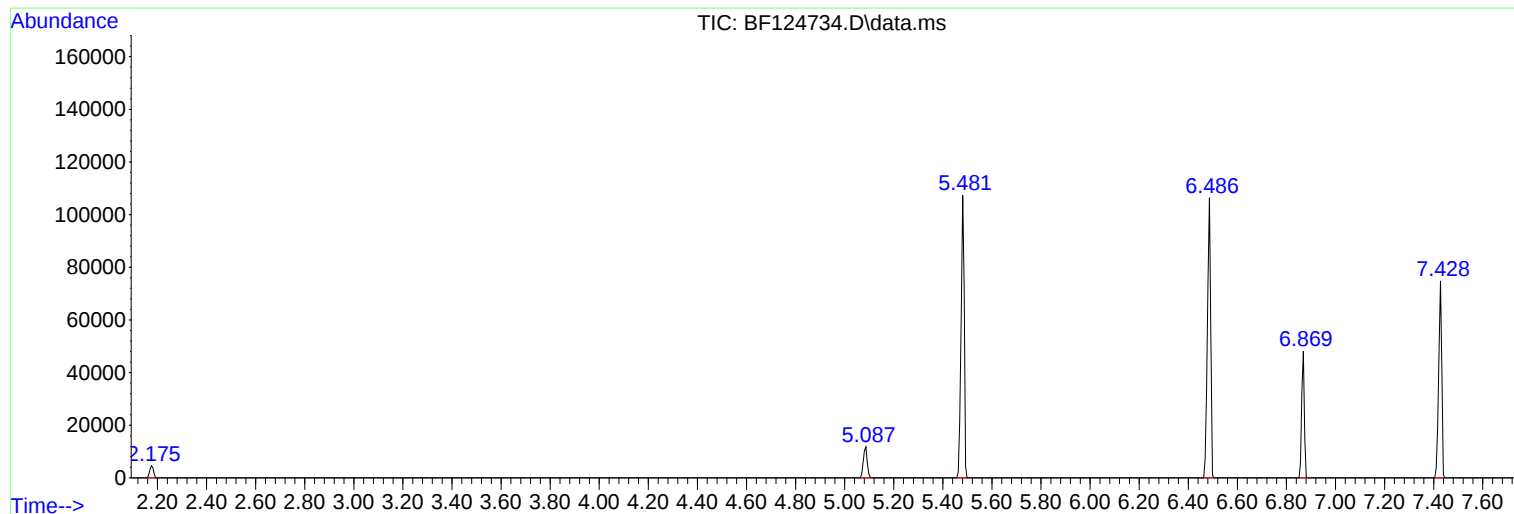
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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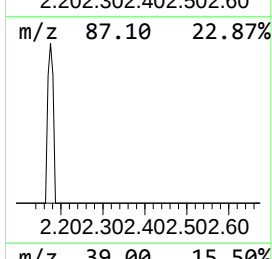
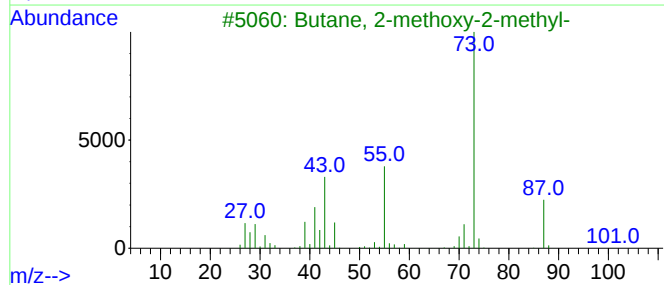
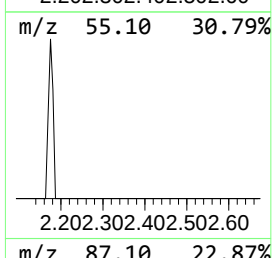
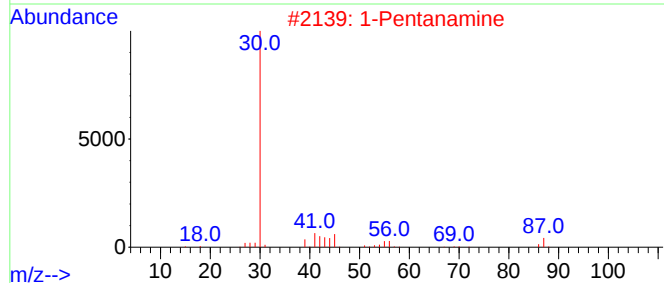
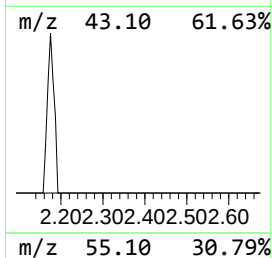
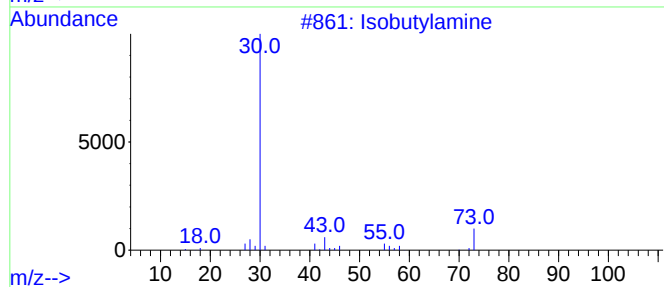
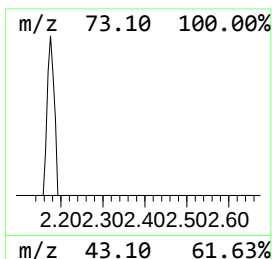
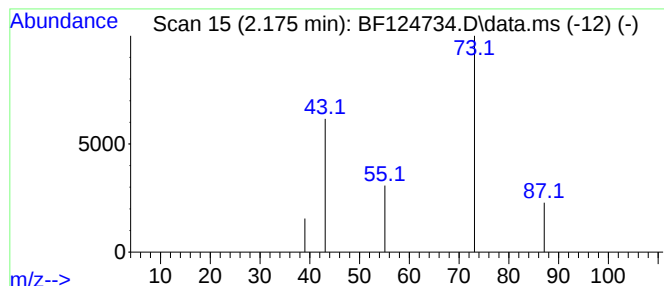
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 unknown2.175 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	2.74 ng	4948	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutylamine	73	C4H11N	000078-81-9	4
2			1-Pentanamine	87	C5H13N	000110-58-7	3
3			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	2
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	2
5			1-Butanamine	73	C4H11N	000109-73-9	2



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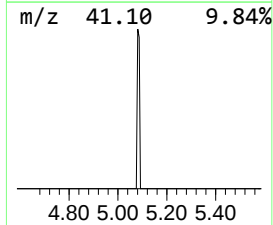
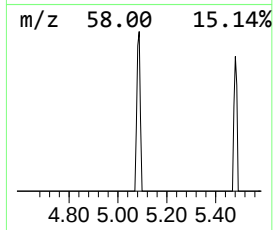
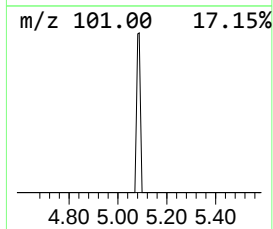
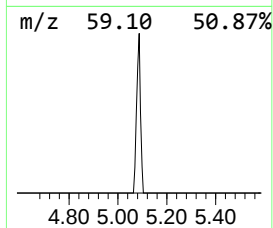
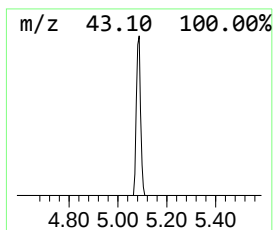
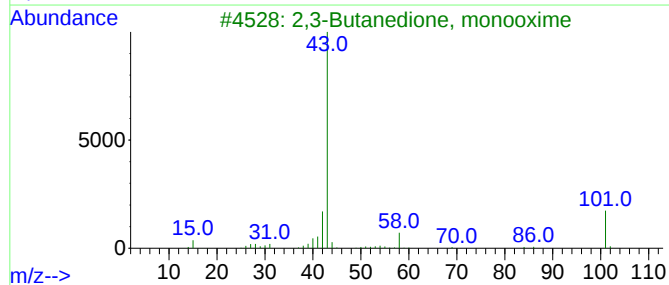
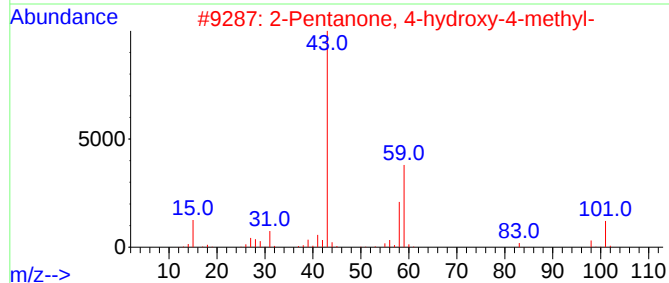
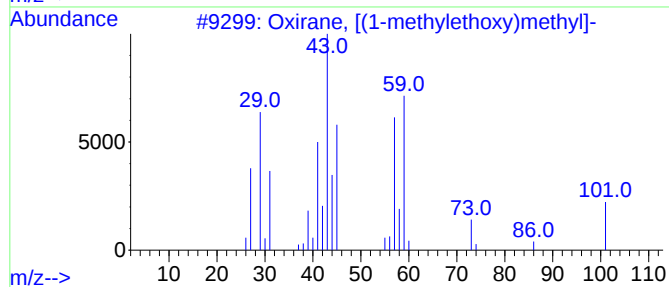
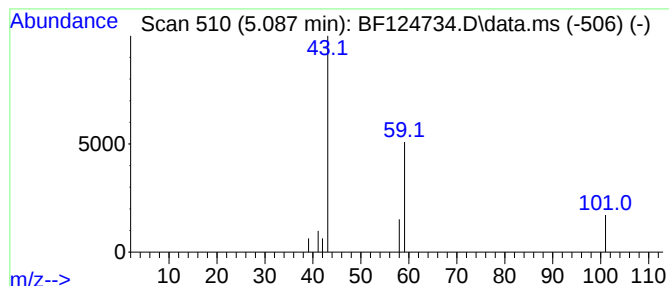
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown5.087 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	7.14 ng	12892	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	9
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
4			Diacetamide	101	C4H7NO2	000625-77-4	7
5			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	5



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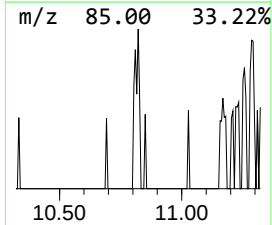
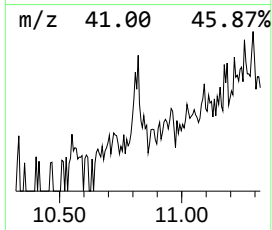
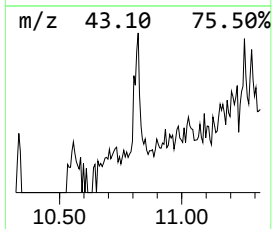
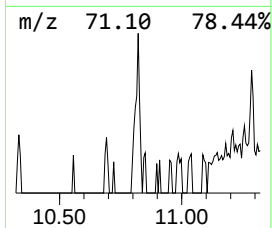
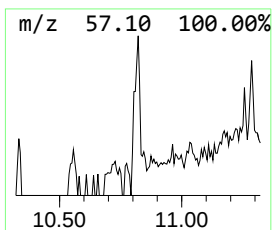
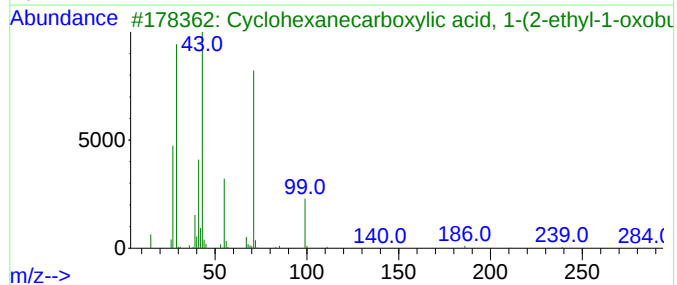
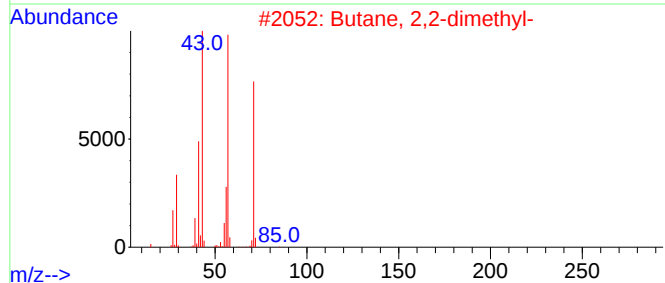
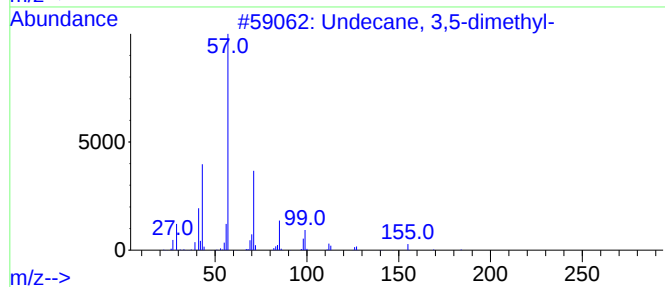
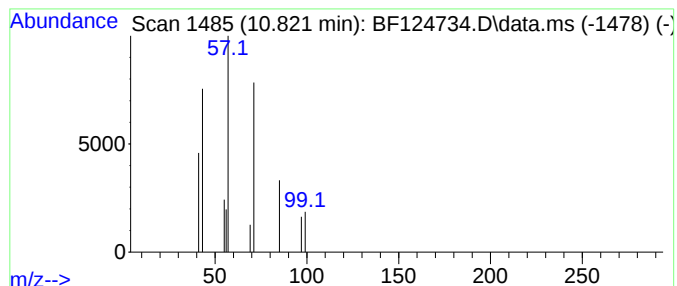
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.822 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	4.43 ng	13947	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	39
2			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
3			Cyclohexanecarboxylic acid, 1-(2...	284	C15H24O5	1000460-66-2	25
4			Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	16
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	12



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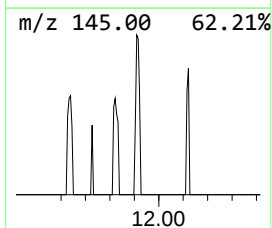
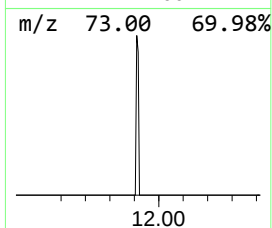
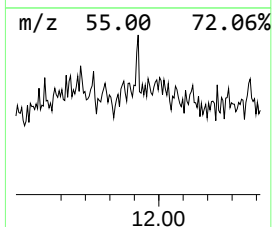
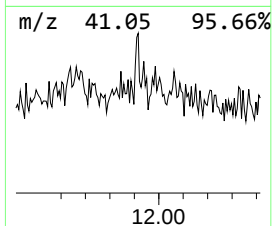
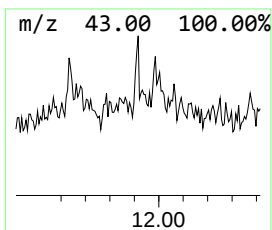
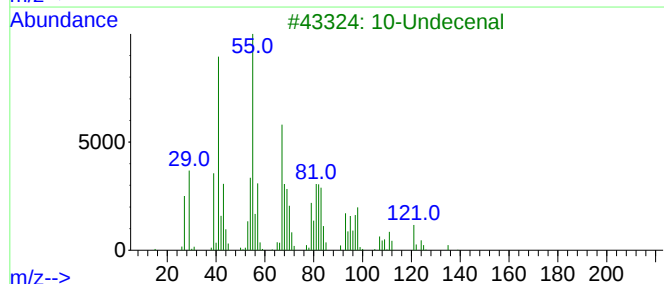
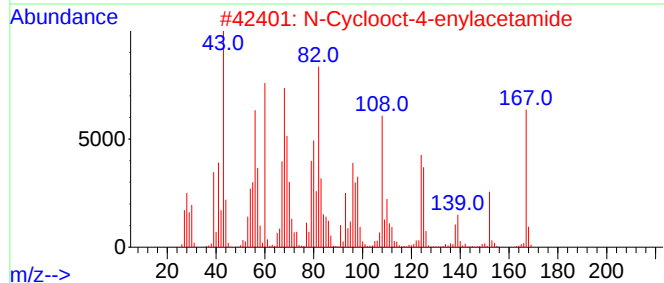
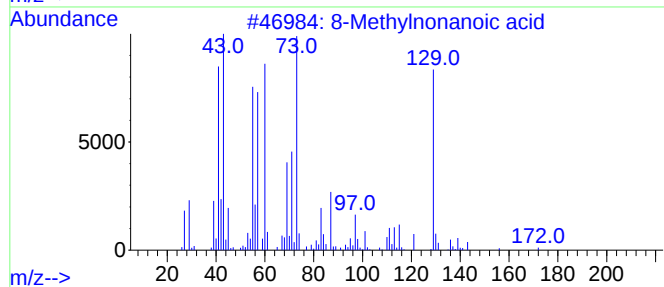
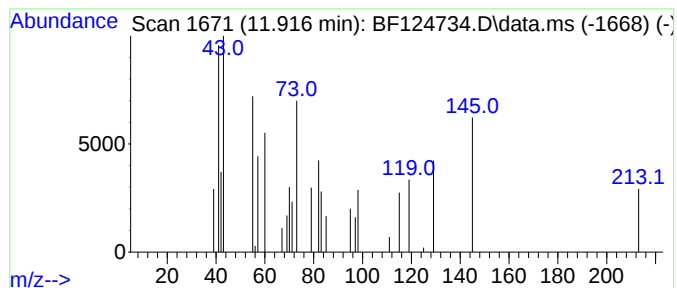
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown11.916 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.71 ng	8536	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	14
2			N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	10
3			10-Undecenal	168	C11H20O	000112-45-8	10
4			n-Decanoic acid	172	C10H20O2	000334-48-5	10
5			1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	10



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ClientSampled :
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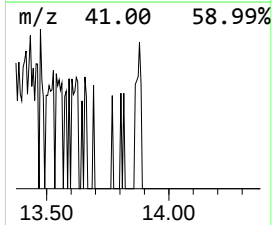
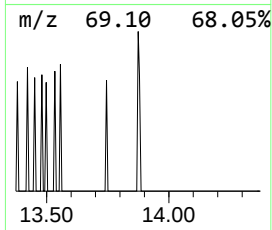
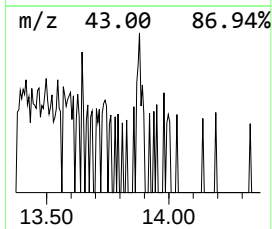
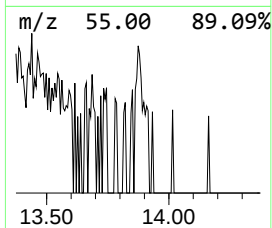
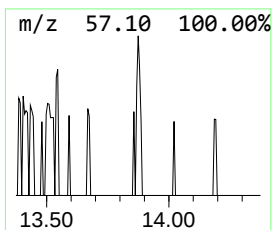
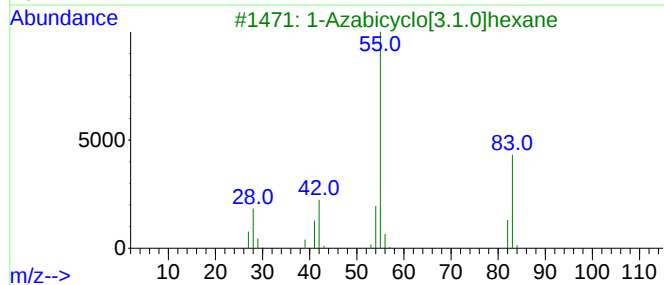
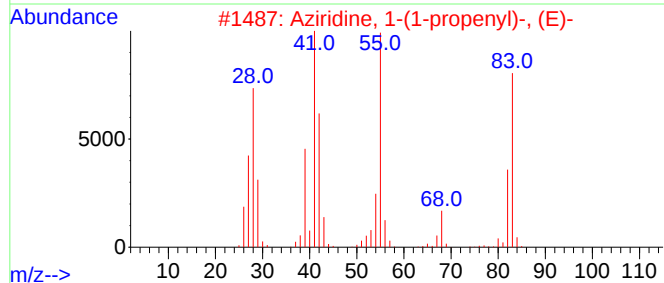
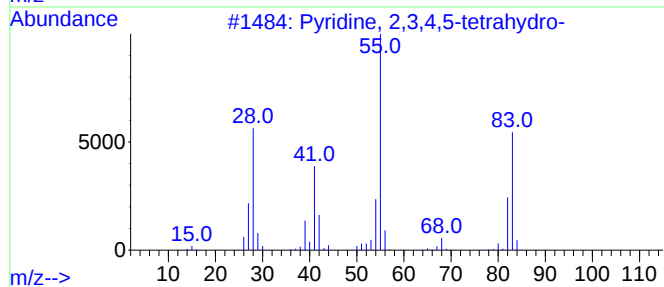
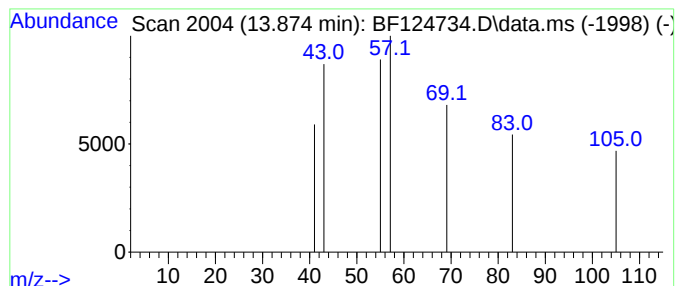
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Peak Number 5 unknown13.874 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.57 ng	5497	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	4
2			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	4
3			1-Azabicyclo[3.1.0]hexane	83	C5H9N	000285-76-7	4
4			Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	4
5			1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072321\
Data File : BF124734.D
Acq On : 24 Jul 2021 2:46
Operator : JU/CG
Sample : M3139-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEW-RO

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.175	2.175	2.7	ng	4948	1	6.869	36121	20.0
unknown5.087	5.087	7.1	ng	12892	1	6.869	36121	20.0
unknown10.822	10.822	4.4	ng	13947	4	11.392	62972	20.0
unknown11.916	11.916	2.7	ng	8536	4	11.392	62972	20.0
unknown13.874	13.874	3.6	ng	5497	5	14.027	30832	20.0