

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
 Data File : BF124843.D
 Acq On : 28 Jul 2021 23:44
 Operator : JU/CG
 Sample : M3174-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-EF-01-021-ABCD

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: BF124843.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	10	rBB	8204	8827	6.12%	0.973%
2	5.087	507	510	513	rBB	2932	2480	1.72%	0.273%
3	5.487	573	578	581	rBB	123519	108071	74.99%	11.911%
4	6.498	745	750	753	rBV	114197	110590	76.74%	12.189%
5	6.869	810	813	816	rBB	46597	33165	23.01%	3.655%
6	7.434	905	909	912	rBB	92956	75151	52.15%	8.283%
7	8.051	1012	1014	1018	rBB	3645	3043	2.11%	0.335%
8	8.151	1028	1031	1034	rBB	54634	42915	29.78%	4.730%
9	9.228	1210	1214	1217	rBV	188438	144118	100.00%	15.884%
10	9.910	1327	1330	1334	rBB	57355	45743	31.74%	5.042%
11	10.698	1460	1464	1467	rBB	74631	63482	44.05%	6.997%
12	11.392	1579	1582	1585	rBV	43320	37706	26.16%	4.156%
13	11.916	1669	1671	1674	rBB	5091	3966	2.75%	0.437%
14	12.604	1786	1788	1791	rBB	5423	4148	2.88%	0.457%
15	12.833	1823	1827	1830	rBB	6468	5466	3.79%	0.602%
16	12.980	1848	1852	1855	rBV	149373	113234	78.57%	12.480%
17	13.892	2003	2007	2017	rVB3	5225	11850	8.22%	1.306%
18	14.033	2025	2031	2034	rBV	38437	35411	24.57%	3.903%
19	14.057	2034	2035	2038	rVB	3780	2853	1.98%	0.314%
20	14.545	2113	2118	2120	rBV3	1675	2099	1.46%	0.231%
21	15.074	2205	2208	2211	rBV2	3170	4590	3.18%	0.506%
22	15.145	2218	2220	2223	rBV3	2893	3142	2.18%	0.346%
23	15.380	2258	2260	2267	rVB2	2391	3790	2.63%	0.418%
24	15.445	2269	2271	2273	rVV2	3283	2811	1.95%	0.310%
25	15.515	2277	2283	2290	rBV	20144	27995	19.43%	3.086%
26	16.074	2374	2378	2380	rBV3	1330	1935	1.34%	0.213%
27	16.221	2400	2403	2408	rVB4	2443	3175	2.20%	0.350%
28	17.251	2574	2578	2581	rBV3	1359	1955	1.36%	0.215%
29	17.545	2626	2628	2633	rBV3	1178	1801	1.25%	0.199%
30	17.715	2655	2657	2662	rVB	1501	1790	1.24%	0.197%

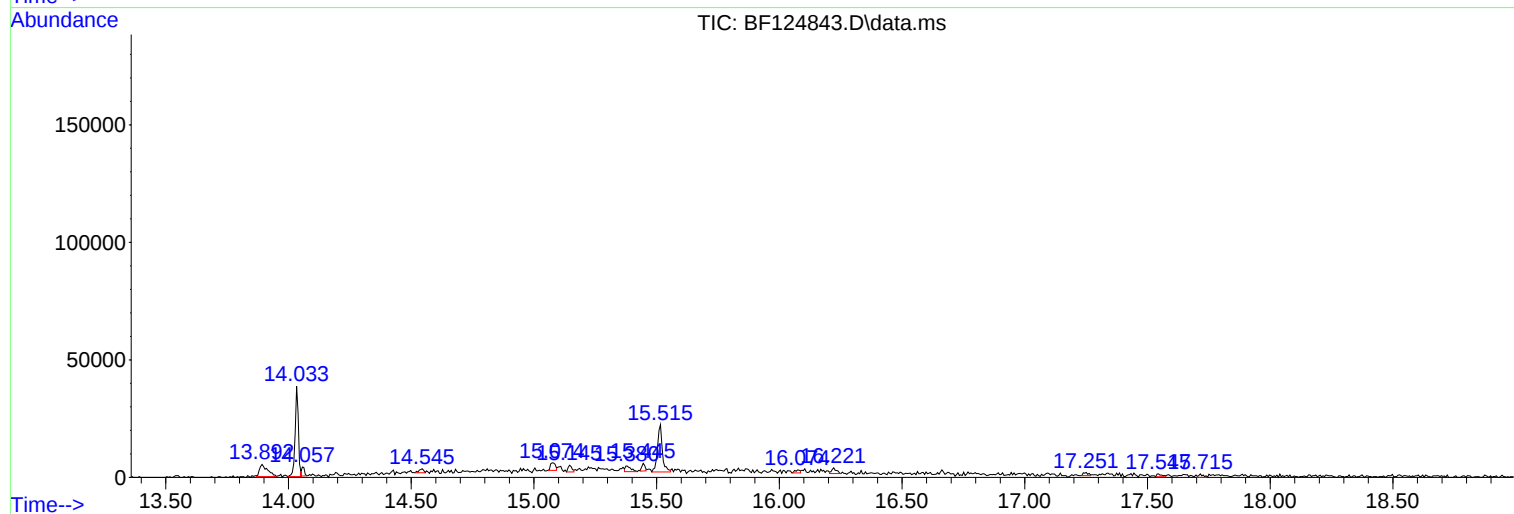
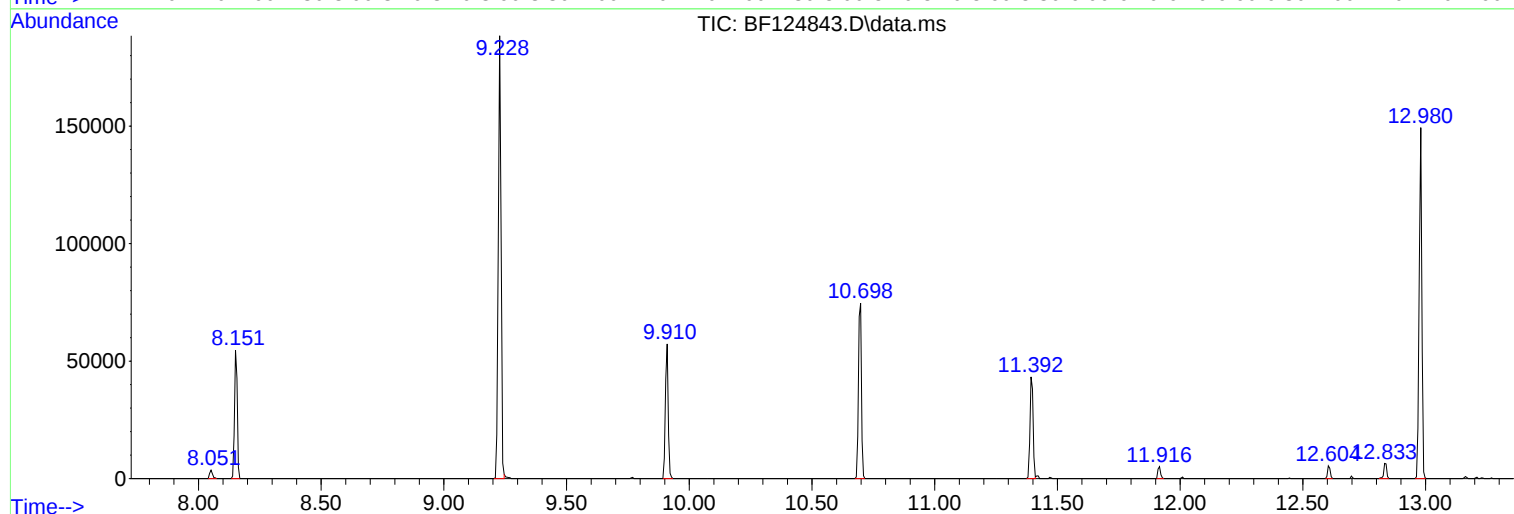
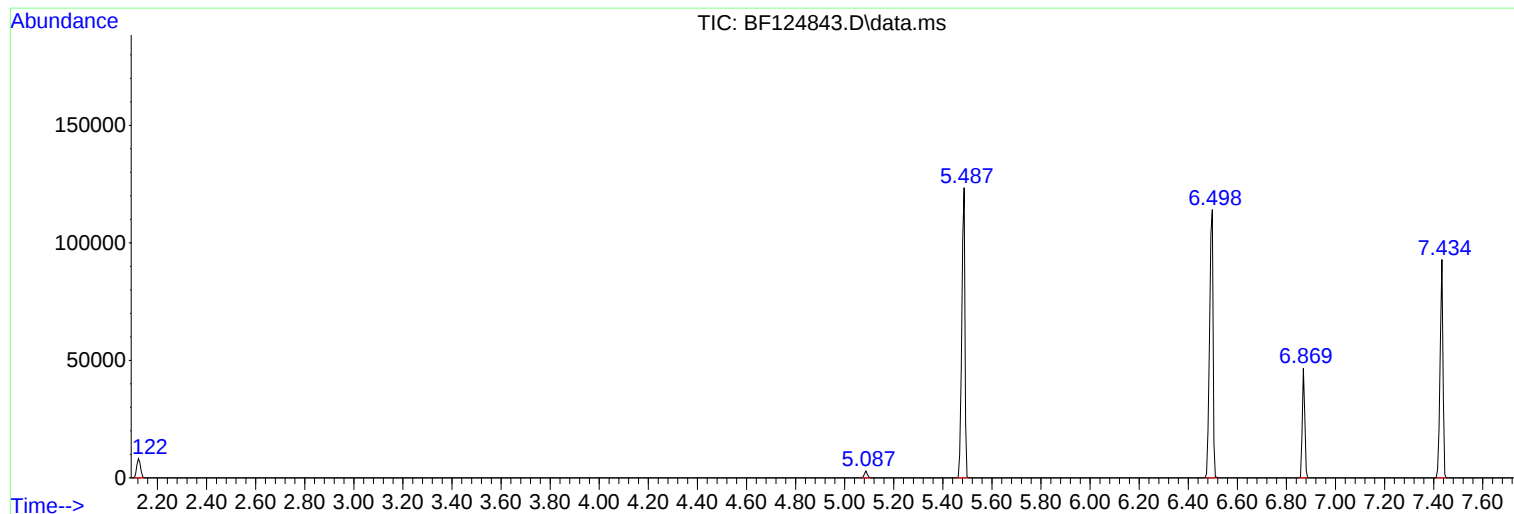
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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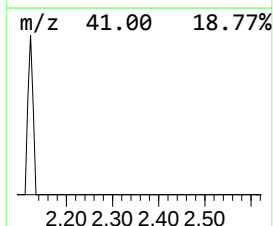
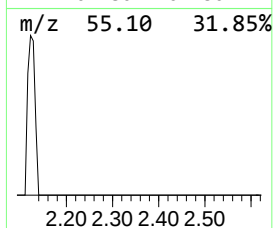
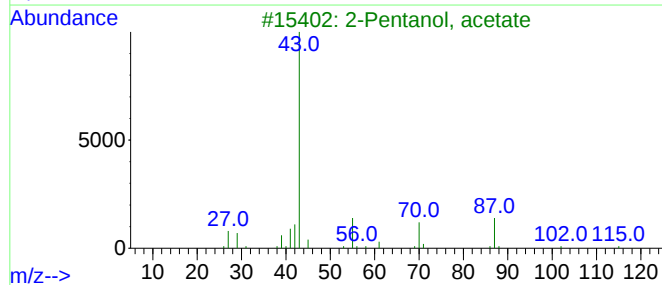
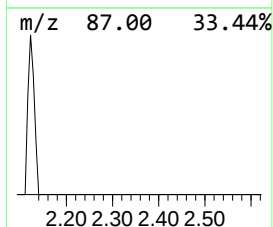
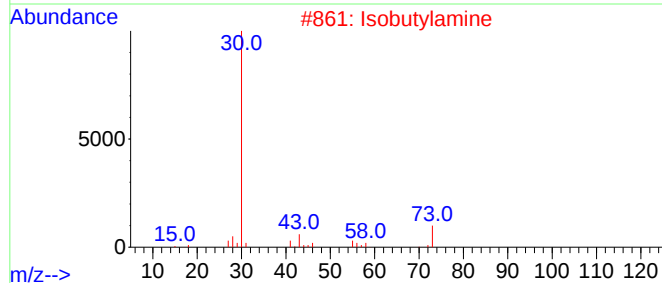
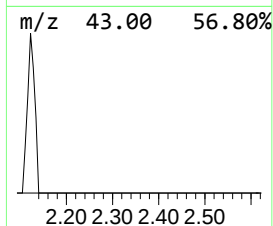
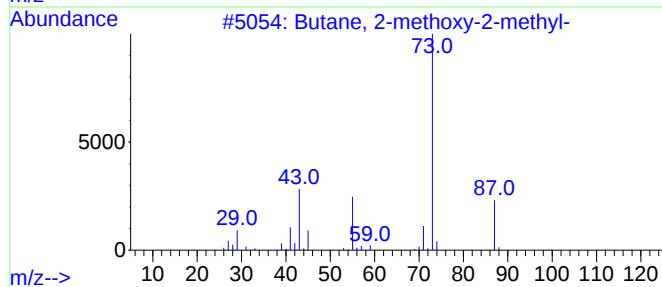
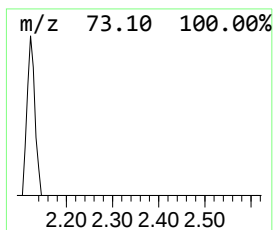
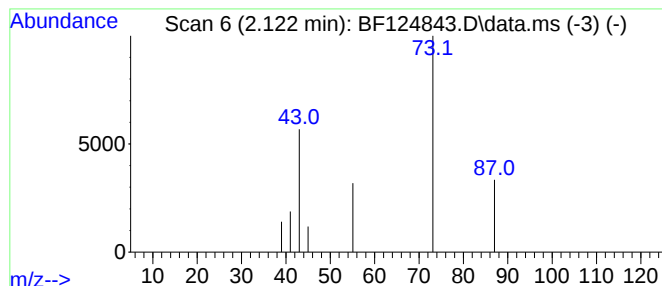
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.122 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	5.32 ng	8827	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			2-Pentanol, acetate	130	C7H14O2	000626-38-0	4
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4



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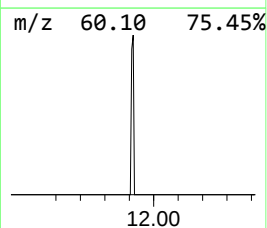
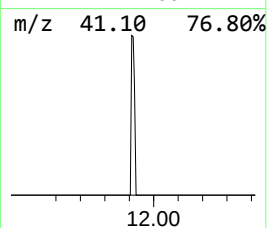
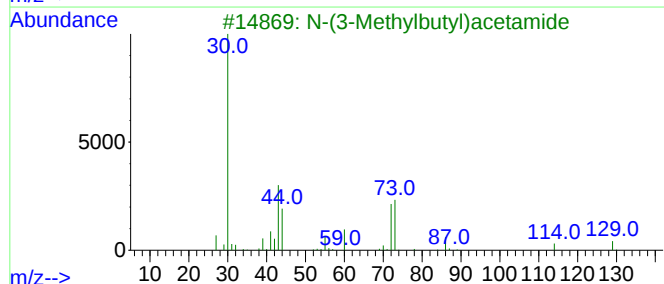
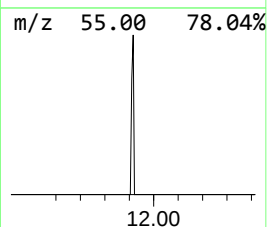
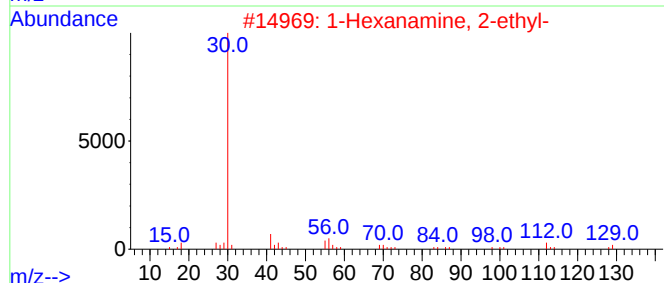
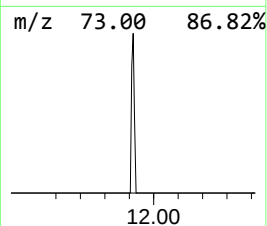
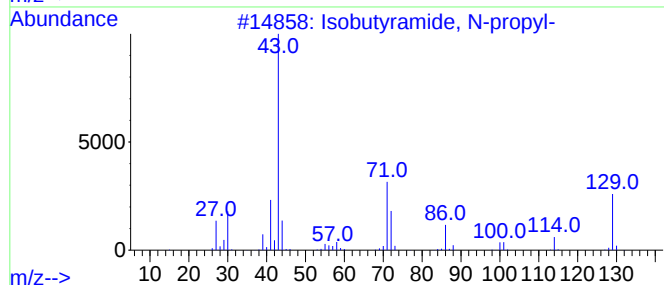
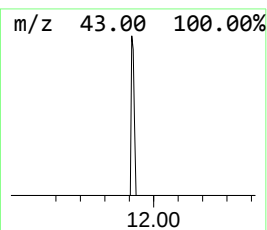
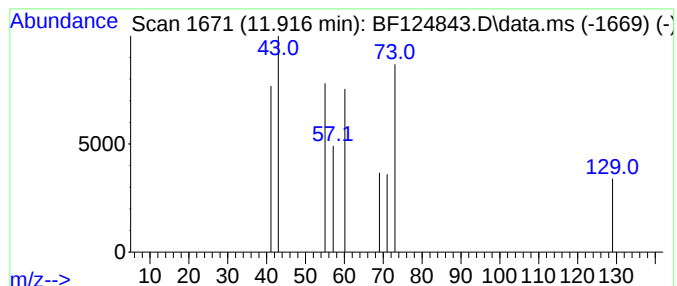
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Peak Number 2 unknown11.916 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.10 ng	3966	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyramide, N-propyl-	129	C7H15NO	1000407-08-5	7
2			1-Hexanamine, 2-ethyl-	129	C8H19N	000104-75-6	5
3			N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	5
4			Acetic acid	60	C2H4O2	000064-19-7	4
5			N-Pentylacetamide	129	C7H15NO	002524-60-9	4



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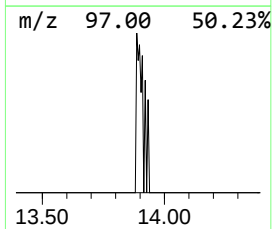
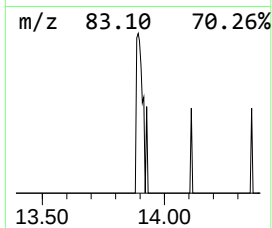
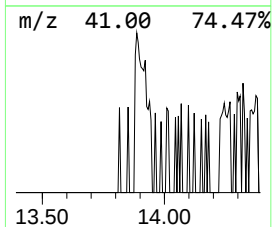
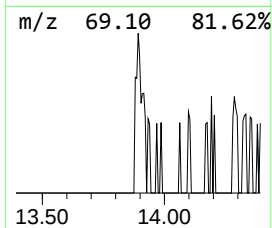
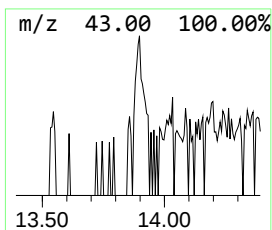
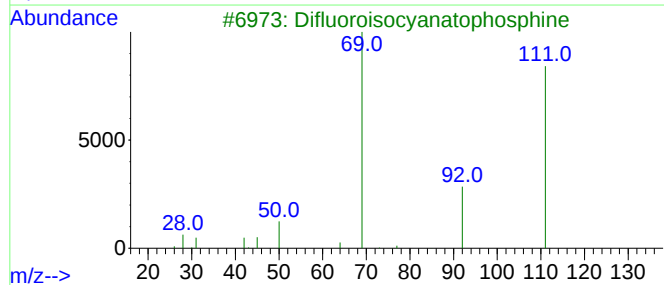
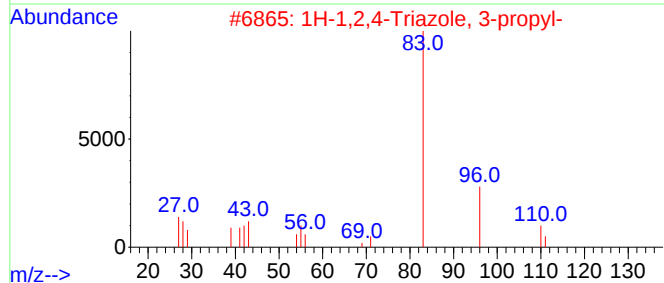
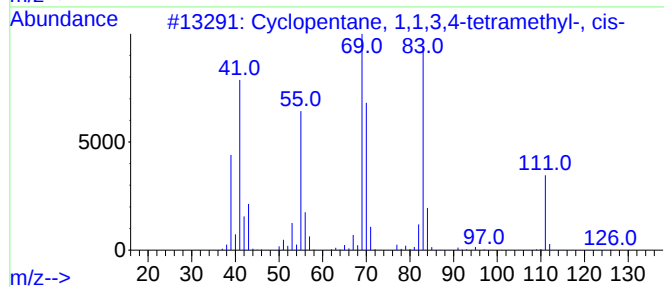
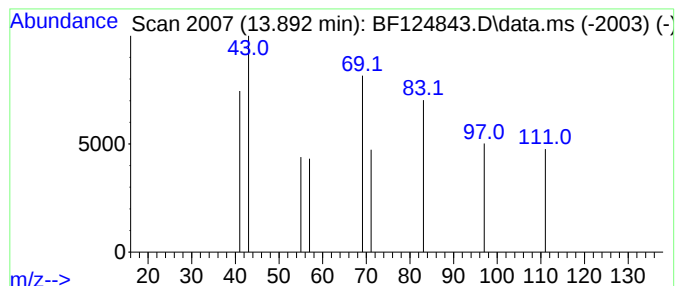
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown13.892 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	6.69 ng	11850	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	053907-60-1	9
2			1H-1,2,4-Triazole, 3-propyl-	111	C5H9N3	019932-60-6	5
3			Difluoroisocyanatophosphine	111	CF2NOP	1000306-12-1	5
4			1-[1,2,4]Triazol-1-ylethanone	111	C4H5N3O	015625-88-4	4
5			2-Hexenal, (E)-	98	C6H10O	006728-26-3	4



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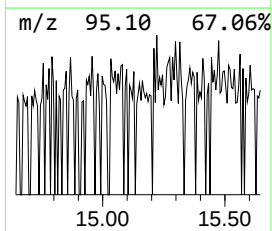
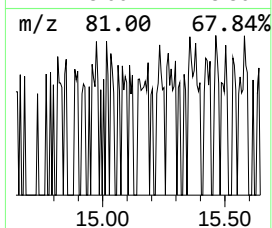
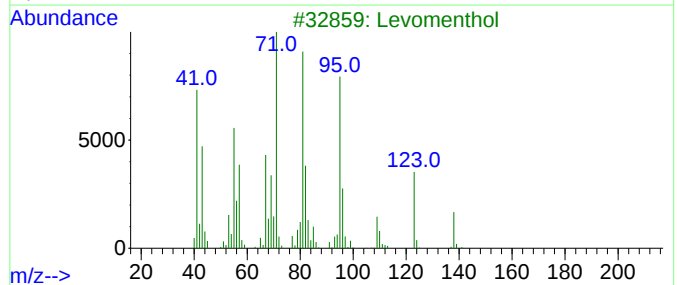
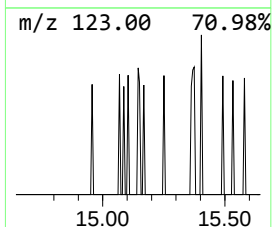
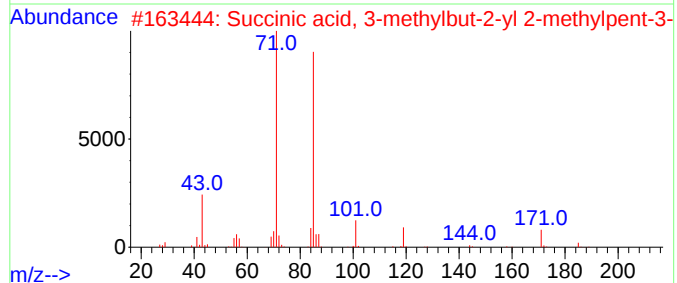
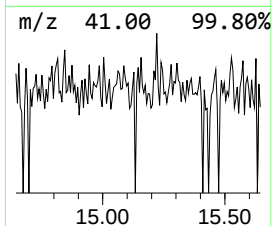
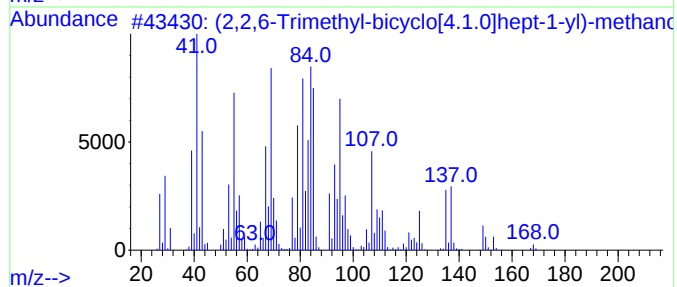
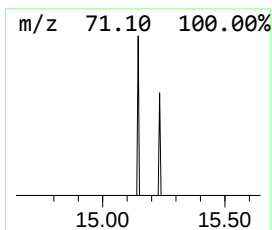
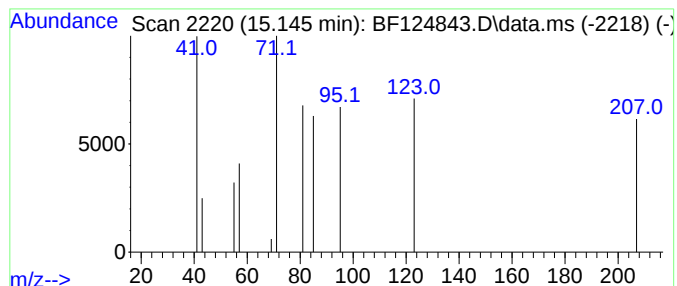
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Peak Number 4 unknown15.145 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	2.24 ng	3142	Perylene-d12	15.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(2,2,6-Trimethyl-bicyclo[4.1.0]h...	168	C11H20O	078996-11-9	10
2		Succinic acid, 3-methylbut-2-yl ...	272	C15H28O4	1000389-59-7	9
3		Levomenthol	156	C10H20O	002216-51-5	9
4		Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	9
5		dl-Menthol	156	C10H20O	000089-78-1	9



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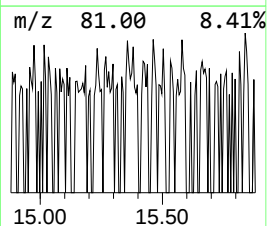
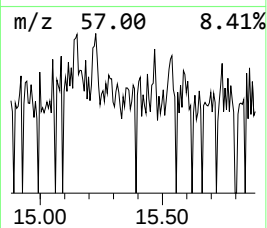
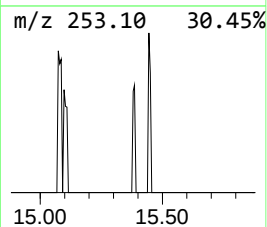
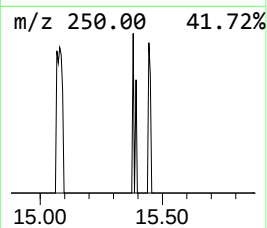
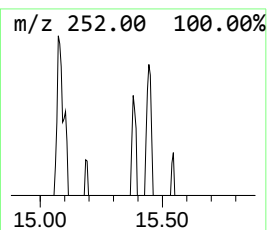
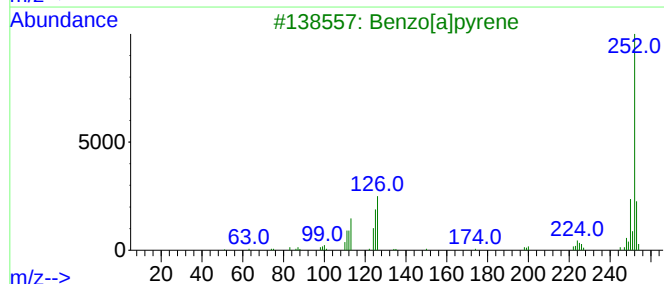
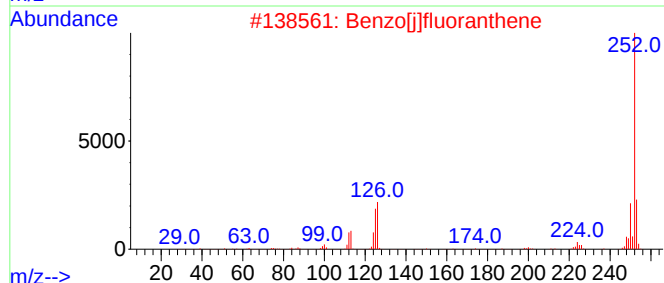
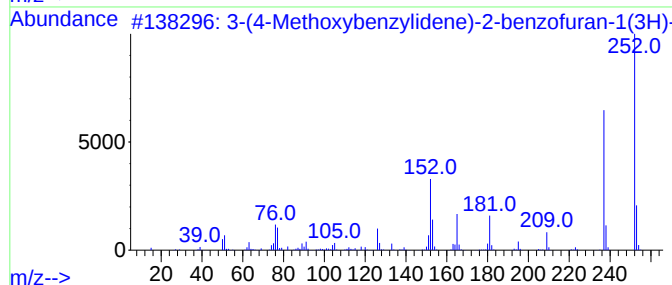
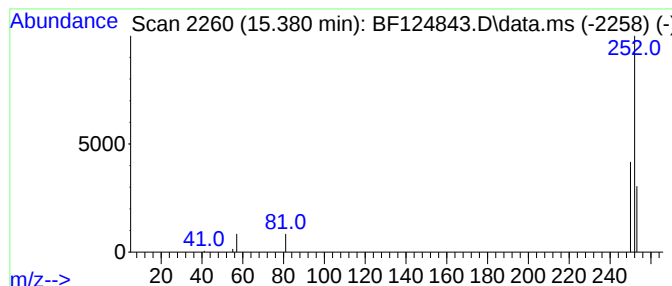
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Peak Number 5 unknown15.380 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	2.71 ng	3790	Perylene-d12	15.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(4-Methoxybenzylidene)-2-benzo...	252	C16H12O3	1000332-19-6	5	
2	Benzo[j]fluoranthene	252	C20H12	000205-82-3	5	
3	Benzo[a]pyrene	252	C20H12	000050-32-8	5	
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	5	
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	5	



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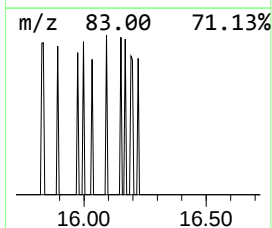
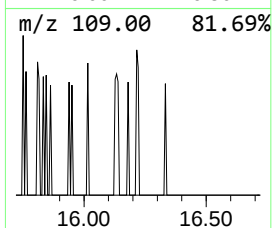
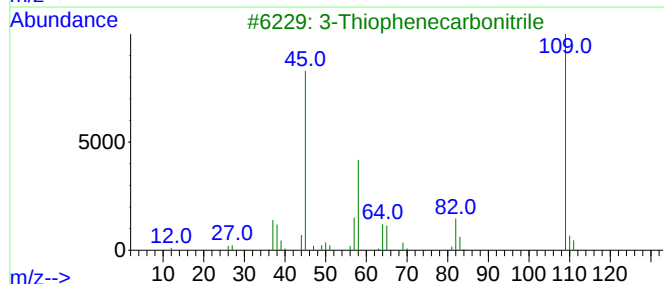
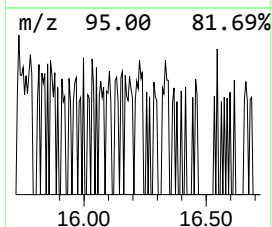
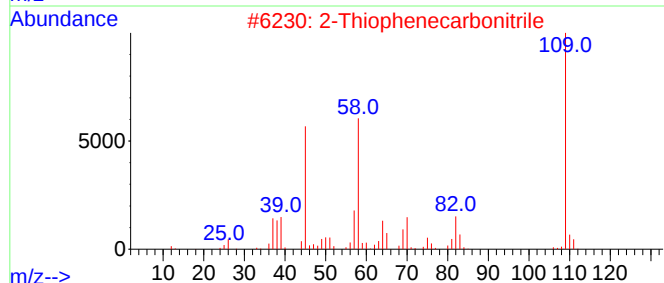
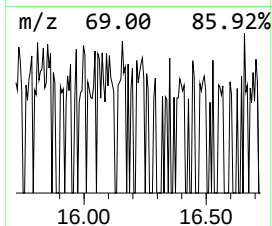
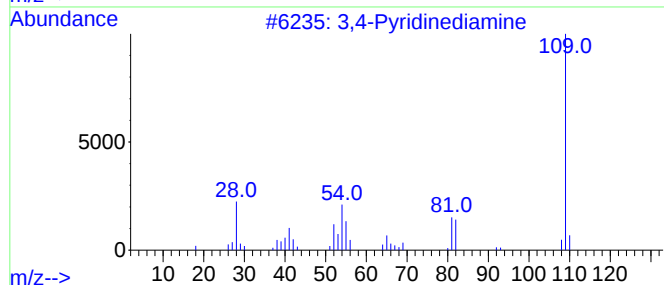
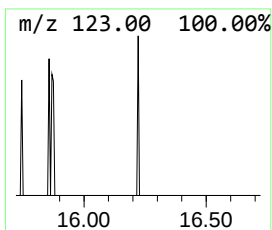
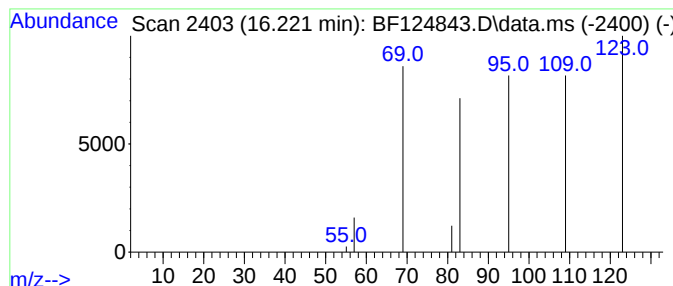
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.221 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.221	2.27 ng	3175	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,4-Pyridinediamine	109	C5H7N3	000054-96-6	4
2			2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	4
3			3-Thiophenecarbonitrile	109	C5H3NS	001641-09-4	4
4			3-Pyridinol, 6-methyl-	109	C6H7NO	001121-78-4	4
5			Phenol, 3-amino-	109	C6H7NO	000591-27-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124843.D
Acq On : 28 Jul 2021 23:44
Operator : JU/CG
Sample : M3174-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-EF-01-021-ABCD

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
unknown2.122	2.122	5.3	ng	8827	1	6.869	33165	20.0
unknown11.916	11.916	2.1	ng	3966	4	11.392	37706	20.0
unknown13.892	13.892	6.7	ng	11850	5	14.033	35411	20.0
unknown15.145	15.145	2.2	ng	3142	6	15.515	27995	20.0
unknown15.380	15.380	2.7	ng	3790	6	15.515	27995	20.0
unknown16.221	16.221	2.3	ng	3175	6	15.515	27995	20.0