

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
 Data File : BF124842.D
 Acq On : 28 Jul 2021 23:11
 Operator : JU/CG
 Sample : M3202-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-02-072721

Integration Parameters: rteint.p

Integrator: RTE

Smoother: 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: BF124842.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	5	8	12	rBB	9389	10933	6.38%	1.022%
2	5.093	508	511	514	rBB	2048	2161	1.26%	0.202%
3	5.487	574	578	581	rBB	144633	129610	75.64%	12.112%
4	6.498	745	750	753	rBV	142056	131686	76.85%	12.306%
5	6.869	810	813	816	rBB	44252	32295	18.85%	3.018%
6	7.434	905	909	912	rBB	103235	88980	51.93%	8.315%
7	8.051	1012	1014	1018	rBB	8227	5964	3.48%	0.557%
8	8.151	1028	1031	1034	rBB	59864	44127	25.75%	4.124%
9	9.228	1210	1214	1217	rBV	222148	171360	100.00%	16.013%
10	9.910	1326	1330	1333	rBB	56267	47428	27.68%	4.432%
11	10.698	1460	1464	1467	rBB	98310	81331	47.46%	7.600%
12	11.392	1579	1582	1585	rBV	49197	40085	23.39%	3.746%
13	11.416	1585	1586	1589	rVB	19776	11755	6.86%	1.098%
14	11.892	1665	1667	1669	rBV	2543	2233	1.30%	0.209%
15	11.916	1669	1671	1674	rVB2	7098	6138	3.58%	0.574%
16	12.004	1684	1686	1689	rBV2	3275	3391	1.98%	0.317%
17	12.604	1786	1788	1791	rBB	13840	12130	7.08%	1.134%
18	12.833	1823	1827	1831	rBB	15175	13445	7.85%	1.256%
19	12.980	1848	1852	1855	rBV	163724	125824	73.43%	11.758%
20	13.163	1878	1883	1885	rBB	1975	2373	1.38%	0.222%
21	13.886	2002	2006	2011	rBV3	4378	9453	5.52%	0.883%
22	14.033	2024	2031	2034	rBV2	37856	35238	20.56%	3.293%
23	14.057	2034	2035	2039	rVB	6225	3739	2.18%	0.349%
24	15.074	2206	2208	2215	rBV2	3118	5593	3.26%	0.523%
25	15.145	2217	2220	2225	rVV3	2052	3016	1.76%	0.282%
26	15.386	2257	2261	2265	rVB2	2488	4274	2.49%	0.399%
27	15.445	2267	2271	2274	rBV	3945	4054	2.37%	0.379%
28	15.510	2274	2282	2288	rBV	23043	28336	16.54%	2.648%
29	15.645	2301	2305	2307	rBV	1627	2554	1.49%	0.239%
30	15.968	2355	2360	2364	rBV2	2706	4745	2.77%	0.443%
31	16.092	2379	2381	2386	rVB3	1893	2667	1.56%	0.249%
32	16.209	2397	2401	2406	rBV3	2201	3188	1.86%	0.298%

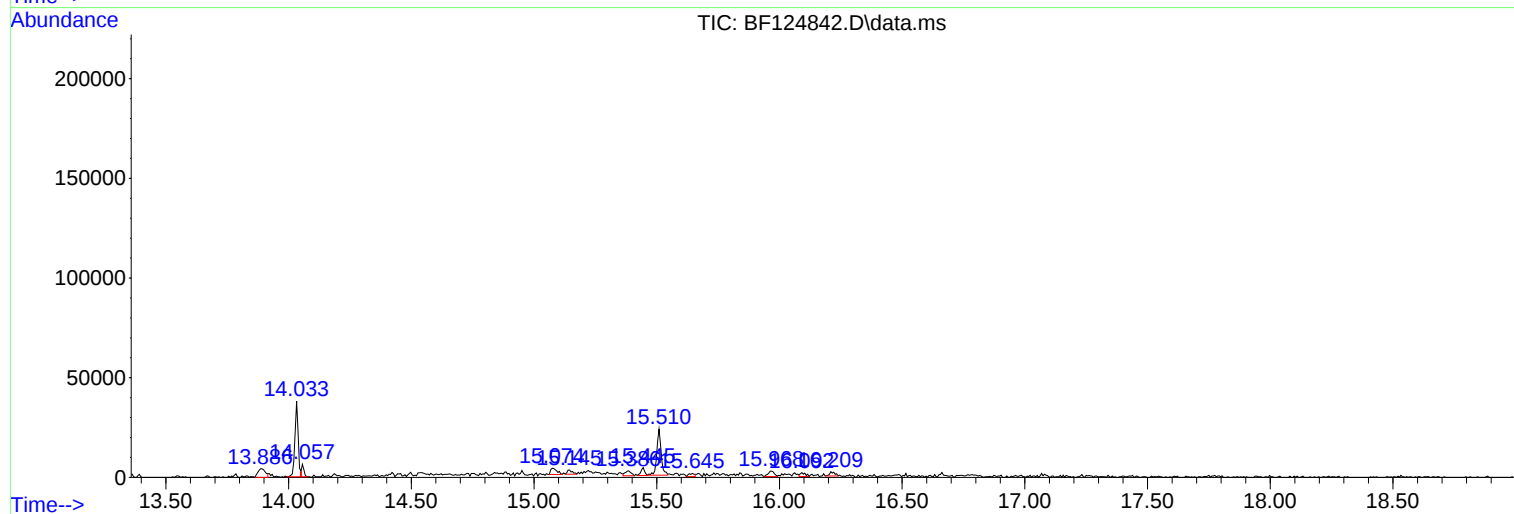
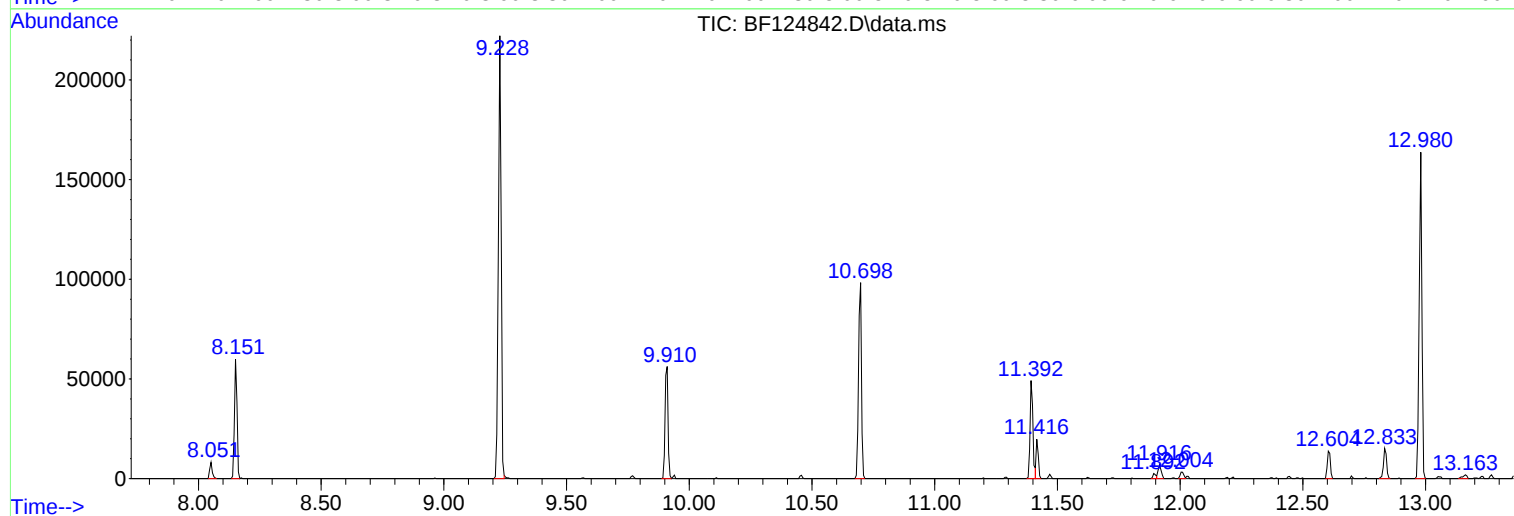
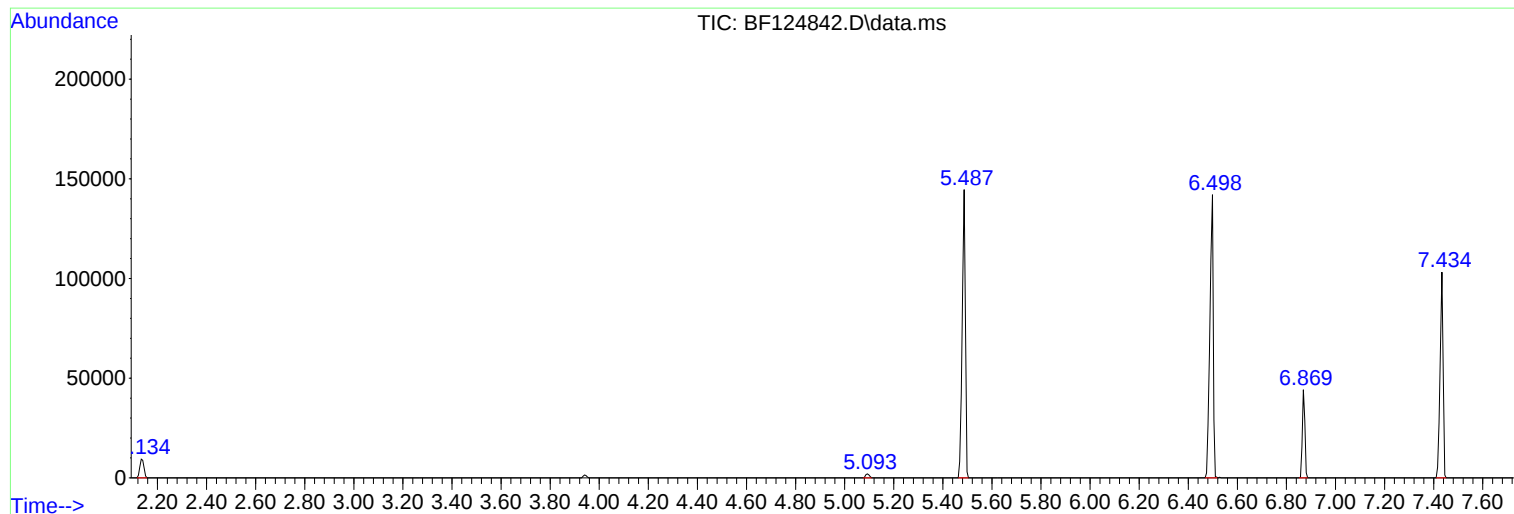
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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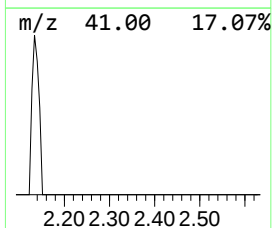
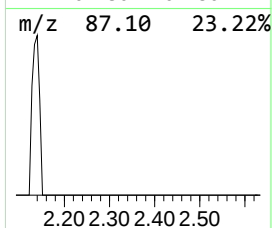
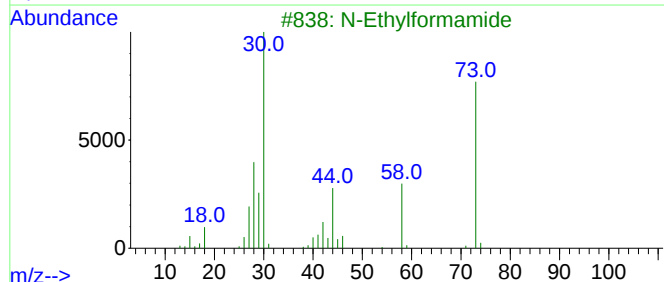
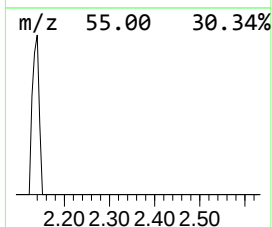
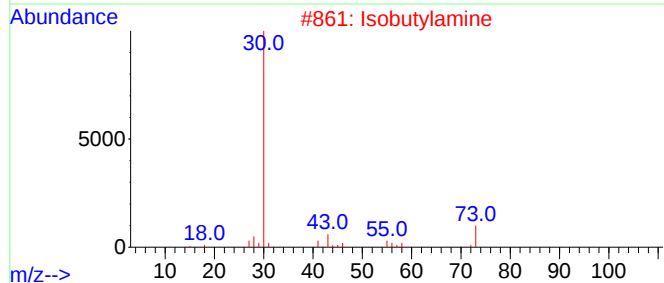
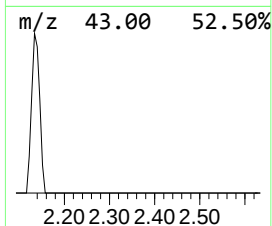
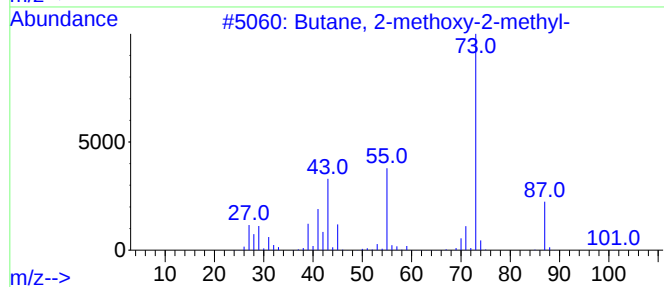
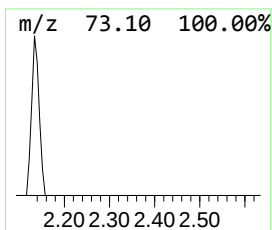
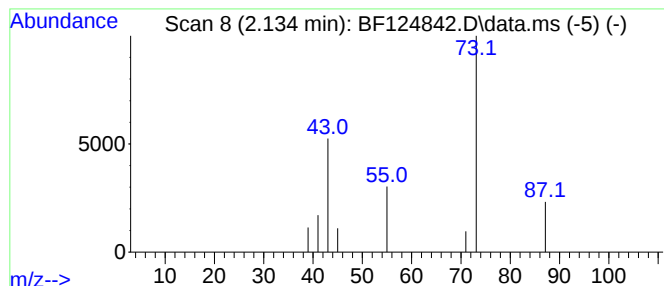
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	6.77 ng	10933	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	74
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			N-Ethylformamide	73	C3H7NO	000627-45-2	4
4			1-Pentanamine	87	C5H13N	000110-58-7	4
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4



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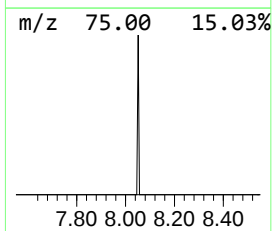
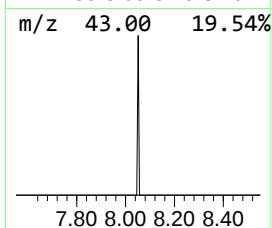
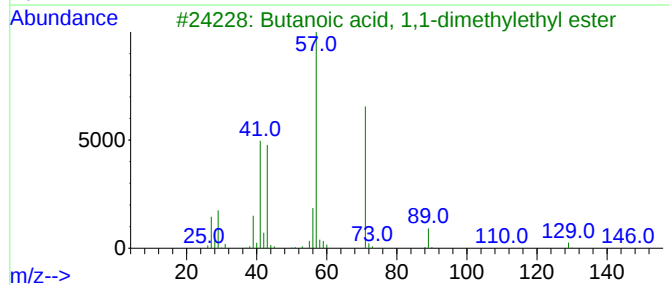
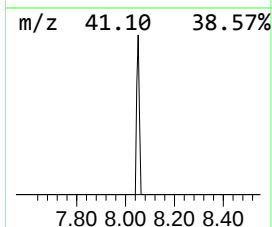
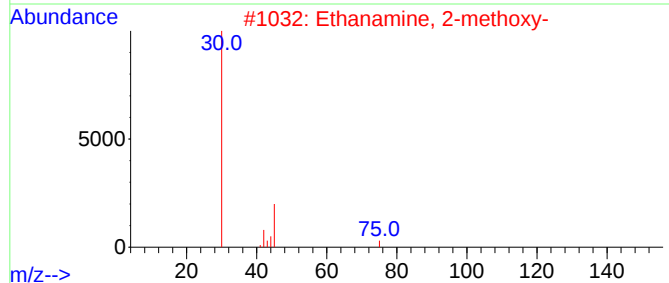
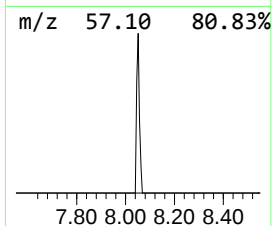
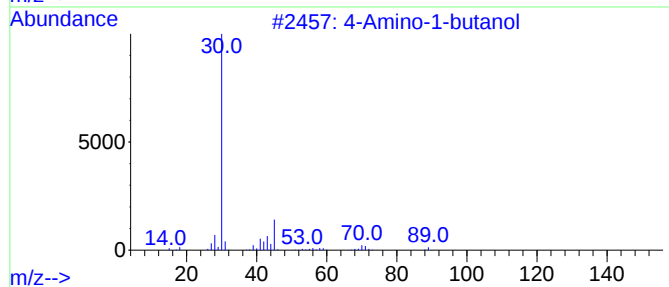
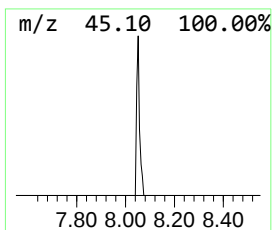
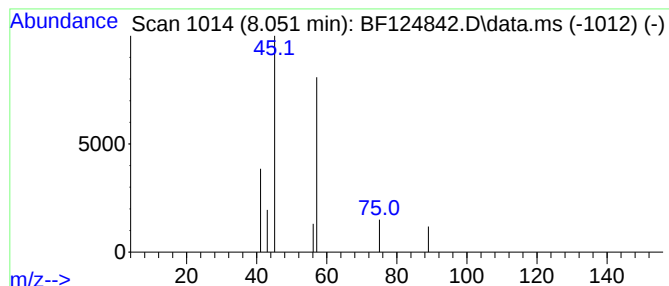
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown8.051 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	2.70 ng	5964	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Amino-1-butanol	89	C4H11NO	013325-10-5	4
2			Ethanamine, 2-methoxy-	75	C3H9NO	000109-85-3	4
3			Butanoic acid, 1,1-dimethylethyl...	144	C8H16O2	002308-38-5	4
4			2-Propanol, 1-amino-, (R)-	75	C3H9NO	002799-16-8	3
5			Formamide	45	CH3NO	000075-12-7	3



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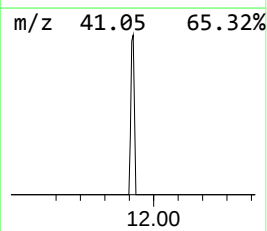
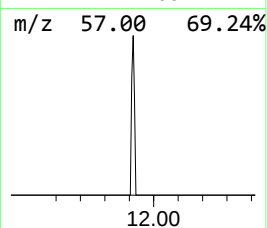
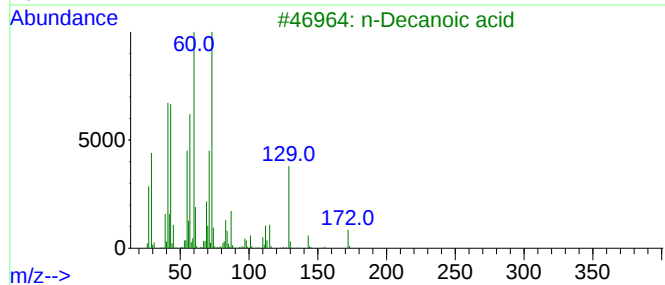
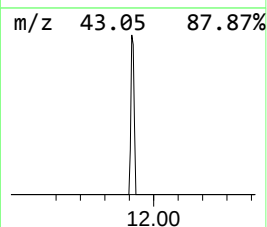
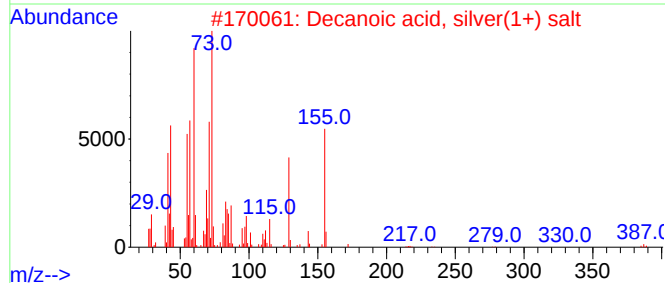
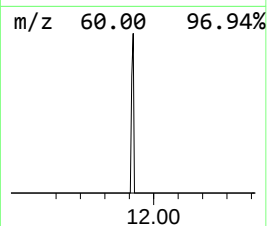
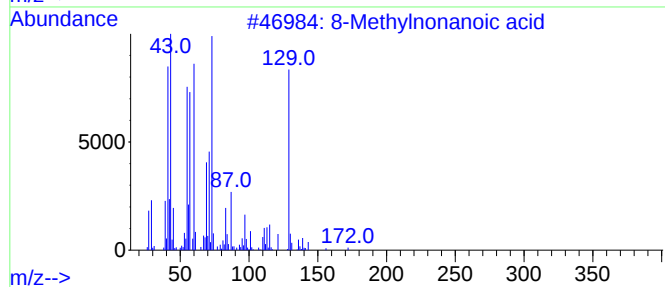
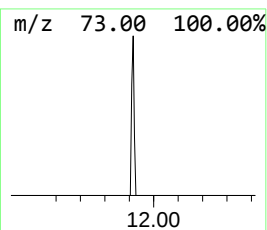
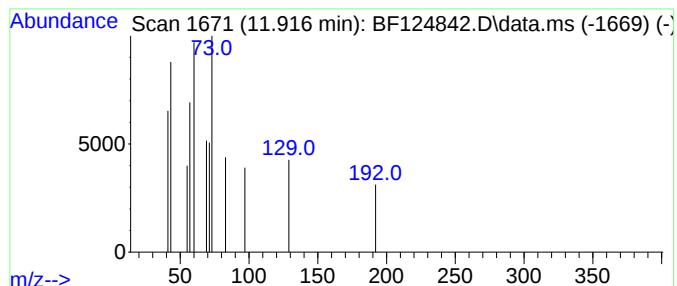
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Peak Number 3 unknown11.916 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.06 ng	6138	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	42
2			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	33
3			n-Decanoic acid	172	C10H20O2	000334-48-5	28
4			Dotriacontyl propyl ether	509	C35H72O	1000406-28-7	25
5			7-Methyloctanoic acid	158	C9H18O2	000693-19-6	23



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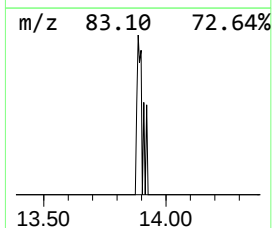
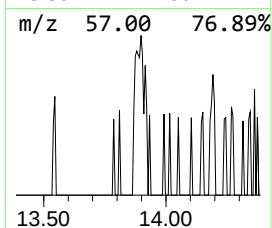
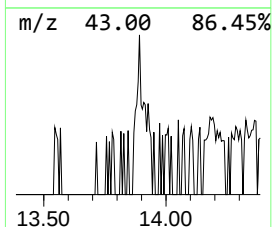
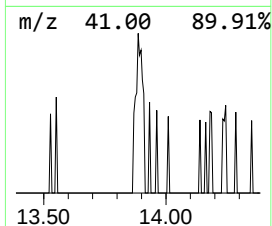
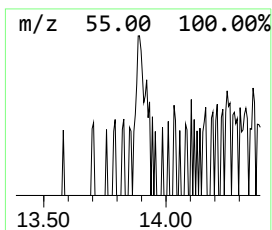
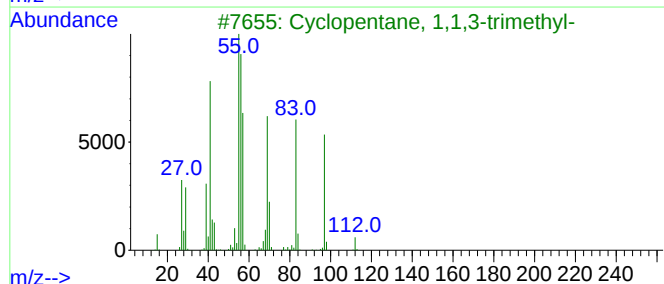
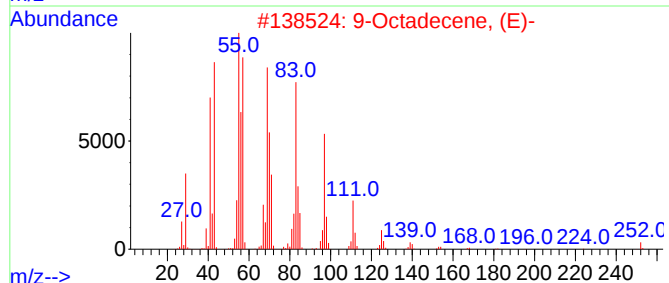
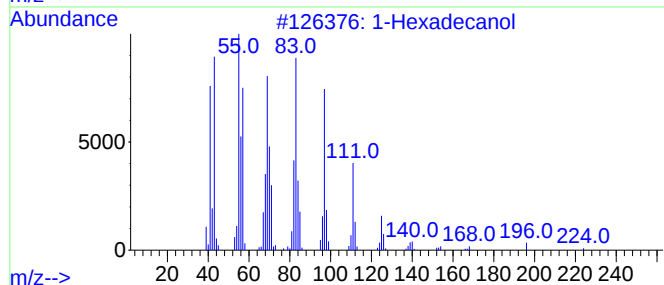
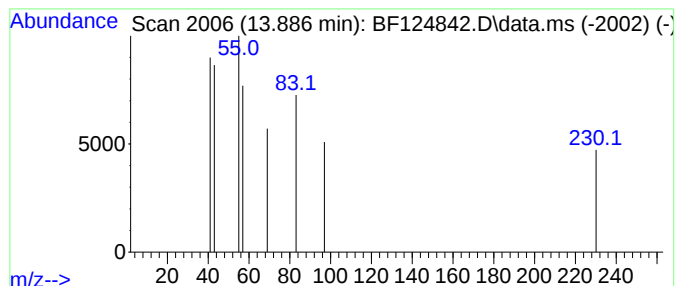
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Peak Number 4 1-Hexadecanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.886	5.37 ng	9453	Chrysene-d12	14.033	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	59
2	9-Octadecene, (E)-	252	C18H36	007206-25-9	59
3	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	59
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	59
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	59



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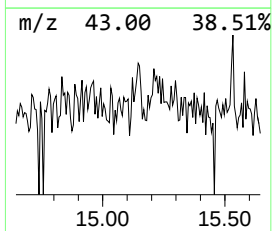
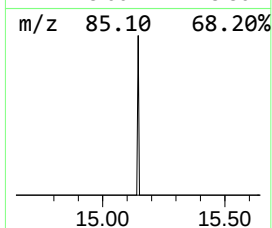
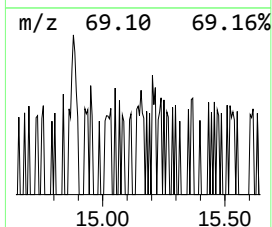
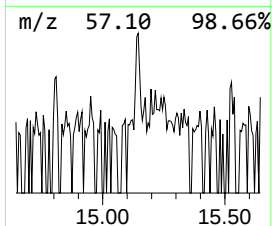
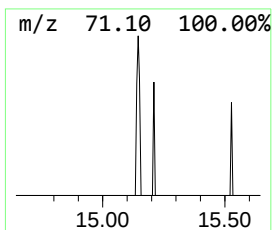
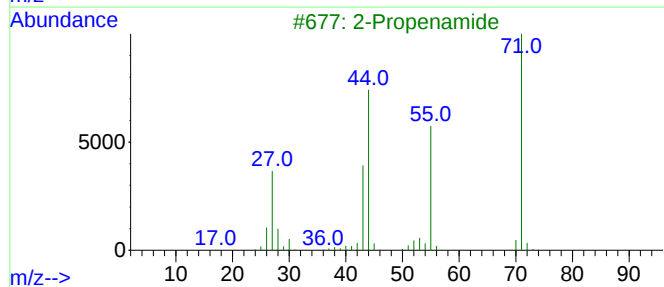
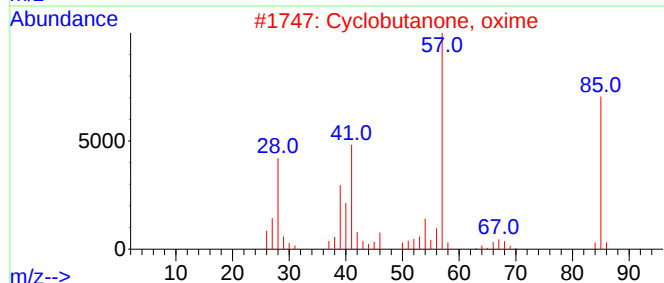
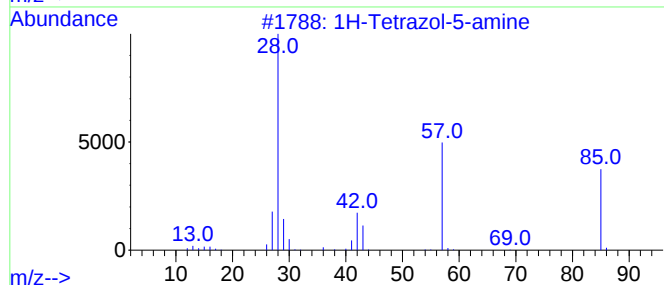
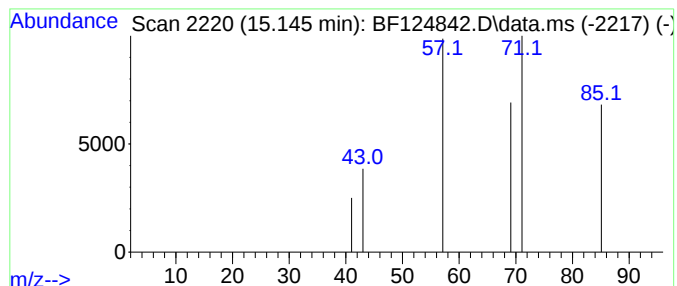
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Peak Number 5 unknown15.145 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	2.13 ng	3016	Perylene-d12	15.509

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4
2		Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
3		2-Propenamide	71	C3H5NO	000079-06-1	4
4		Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	3
5		Isothiazole	85	C3H3NS	000288-16-4	2



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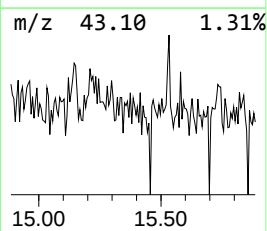
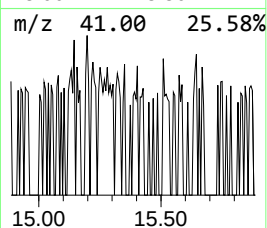
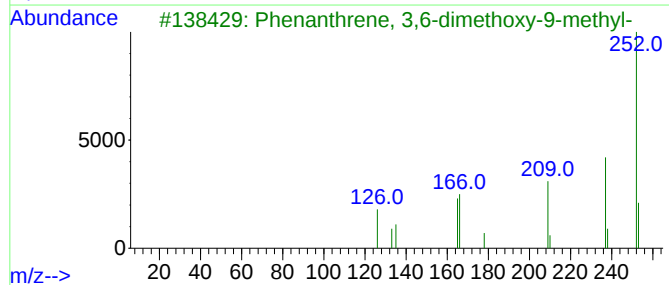
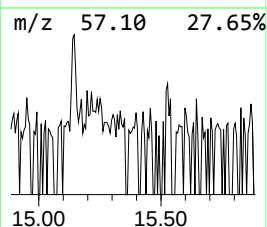
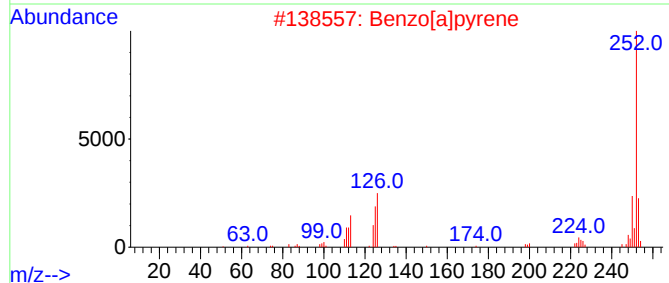
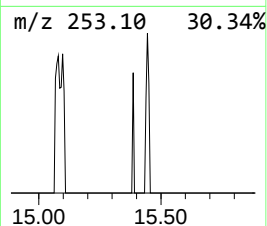
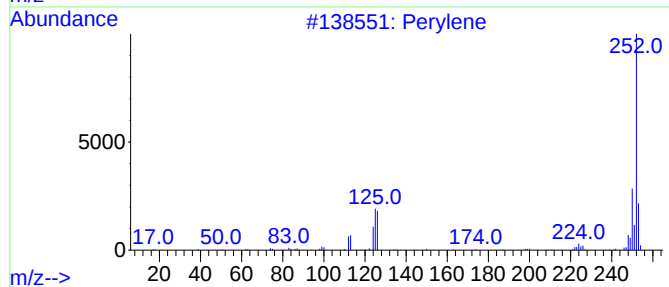
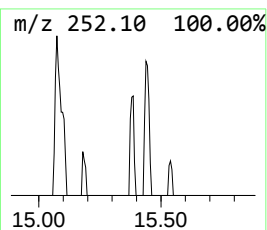
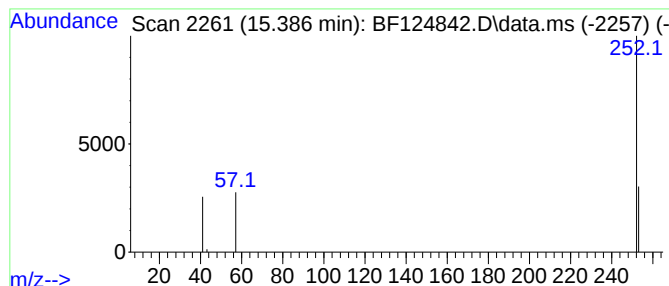
Instrument :
BNA_F
ClientSampleId :
CL-02-072721

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 6 unknown15.386 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.386	3.02 ng	4274	Perylene-d12		15.509	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Perylene		252	C20H12	000198-55-0	5
2	Benzo[a]pyrene		252	C20H12	000050-32-8	5
3	Phenanthrene, 3,6-dimethoxy-9-me...		252	C17H16O2	015638-09-2	5
4	Benzo[k]fluoranthene		252	C20H12	000207-08-9	5
5	1-Phenyl-3-(4-methoxyphenyl)-2-p...		252	C16H16N2O	003314-43-0	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124842.D
Acq On : 28 Jul 2021 23:11
Operator : JU/CG
Sample : M3202-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-072721

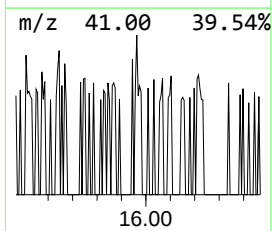
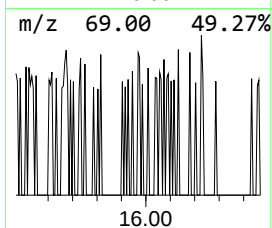
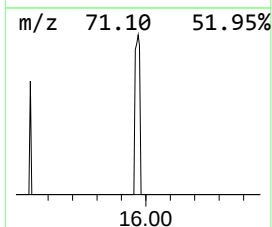
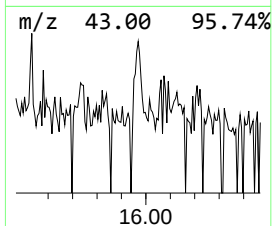
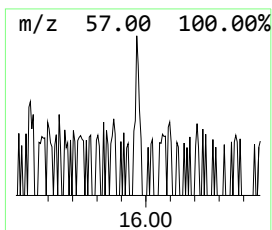
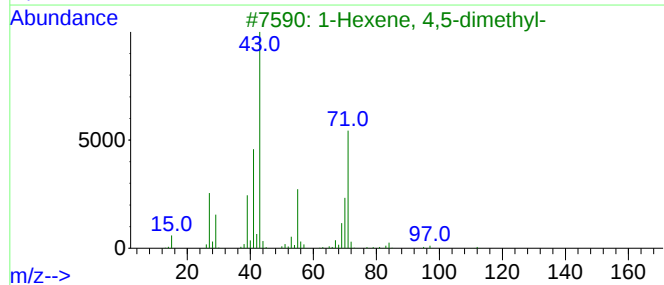
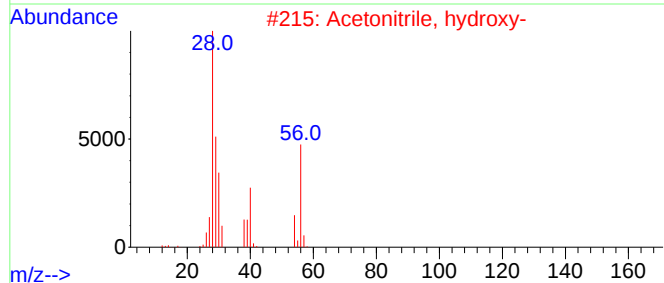
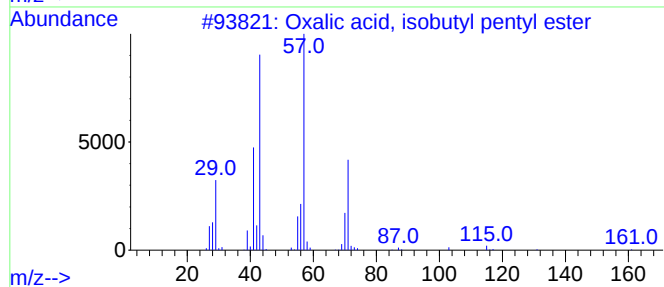
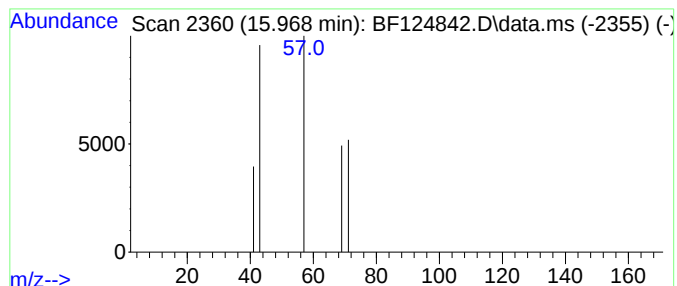
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.968 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	3.35 ng	4745	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	4
2			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
3			1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	2
4			2-Propenamide	71	C3H5NO	000079-06-1	2
5			Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124842.D
Acq On : 28 Jul 2021 23:11
Operator : JU/CG
Sample : M3202-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-072721

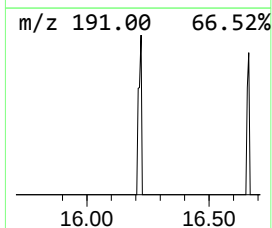
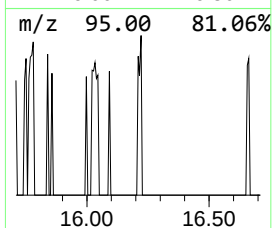
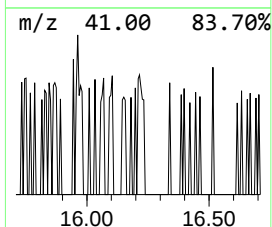
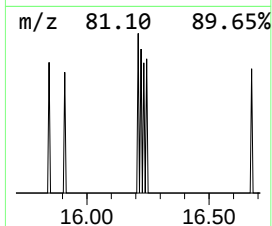
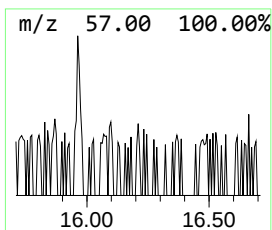
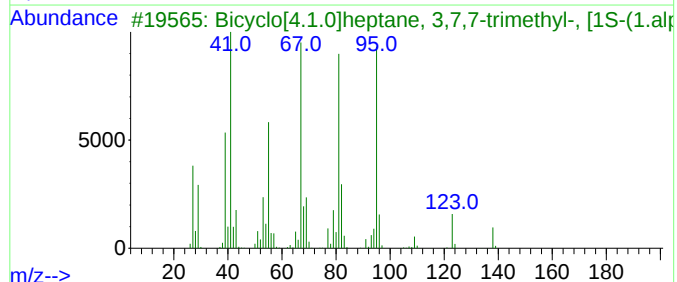
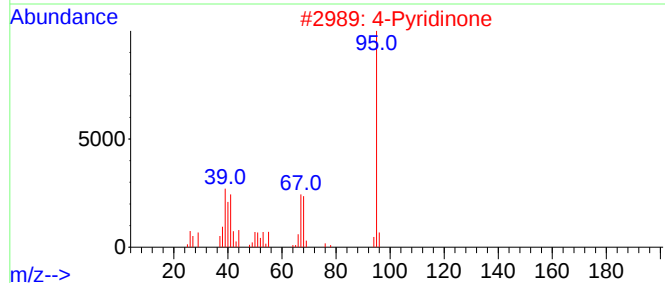
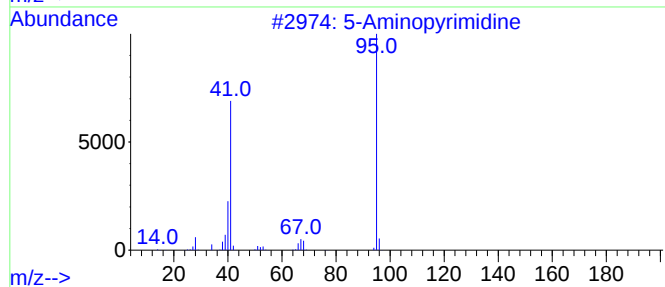
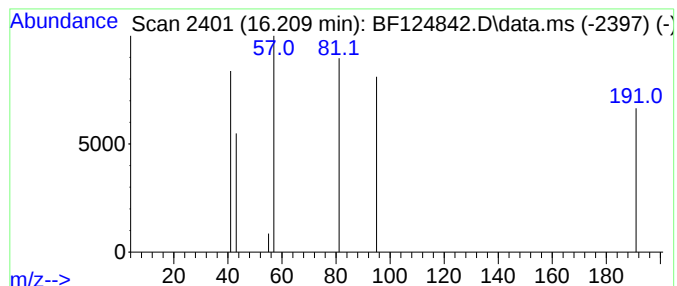
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.209 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.209	2.25 ng	3188	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Aminopyrimidine	95	C4H5N3	000591-55-9	4
2			4-Pyridinone	95	C5H5NO	1000433-50-4	4
3			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	006069-97-2	4
4			3-Pyridinol	95	C5H5NO	000109-00-2	4
5			4-Pyridinol	95	C5H5NO	000626-64-2	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
Data File : BF124842.D
Acq On : 28 Jul 2021 23:11
Operator : JU/CG
Sample : M3202-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-072721

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.134	6.8	ng	10933	1	6.869	32295	20.0
unknown8.051	8.051	2.7	ng	5964	2	8.151	44127	20.0
unknown11.916	11.916	3.1	ng	6138	4	11.392	40085	20.0
1-Hexadecanol	13.886	5.4	ng	9453	5	14.033	35238	20.0
unknown15.145	15.145	2.1	ng	3016	6	15.509	28336	20.0
unknown15.386	15.386	3.0	ng	4274	6	15.509	28336	20.0
unknown15.968	15.968	3.4	ng	4745	6	15.509	28336	20.0
unknown16.209	16.209	2.3	ng	3188	6	15.509	28336	20.0