

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
 Data File : BF124881.D
 Acq On : 30 Jul 2021 17:52
 Operator : JU/CG
 Sample : M3238-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 221

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: BF124881.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	9	rVB	10072	10304	4.66%	0.636%
2	5.092	508	511	515	rBB	3544	3838	1.74%	0.237%
3	5.487	574	578	581	rBV	156240	150169	67.97%	9.273%
4	6.498	745	750	753	rBV	146916	159733	72.29%	9.864%
5	6.869	810	813	816	rBB	47067	33772	15.29%	2.086%
6	7.434	905	909	912	rBV	117714	109068	49.36%	6.735%
7	8.051	1011	1014	1022	rBB	42173	32819	14.85%	2.027%
8	8.151	1028	1031	1034	rBV	63263	48909	22.14%	3.020%
9	9.228	1210	1214	1217	rBV	249654	220947	100.00%	13.644%
10	9.910	1326	1330	1333	rBV	77530	62643	28.35%	3.868%
11	10.704	1461	1465	1468	rBV	150685	143127	64.78%	8.839%
12	11.398	1579	1583	1585	rBV	79054	63207	28.61%	3.903%
13	11.421	1585	1587	1590	rVB	19582	14585	6.60%	0.901%
14	11.921	1669	1672	1675	rVB2	12527	11267	5.10%	0.696%
15	12.010	1684	1687	1689	rBB2	3325	2710	1.23%	0.167%
16	12.610	1786	1789	1792	rBB	25794	19601	8.87%	1.210%
17	12.839	1823	1828	1831	rBB	18412	16310	7.38%	1.007%
18	12.986	1848	1853	1856	rBV	243446	209891	95.00%	12.961%
19	13.874	2002	2004	2013	rBB	12472	17056	7.72%	1.053%
20	14.010	2024	2027	2030	rBV	178757	170432	77.14%	10.525%
21	14.039	2030	2032	2034	rVV	37008	30105	13.63%	1.859%
22	14.062	2034	2036	2038	rVB	4087	3375	1.53%	0.208%
23	14.492	2107	2109	2112	rBV	2676	2918	1.32%	0.180%
24	14.621	2126	2131	2134	rVB3	1751	3077	1.39%	0.190%
25	14.657	2134	2137	2141	rBV	33601	27615	12.50%	1.705%
26	14.804	2155	2162	2166	rBV2	5031	7754	3.51%	0.479%
27	14.892	2173	2177	2181	rBV3	2403	3124	1.41%	0.193%
28	15.080	2206	2209	2212	rBV2	4528	5799	2.62%	0.358%
29	15.145	2217	2220	2223	rBB	3064	2738	1.24%	0.169%
30	15.451	2269	2272	2275	rBB	2675	2463	1.11%	0.152%
31	15.515	2279	2283	2289	rBB	24674	30002	13.58%	1.853%

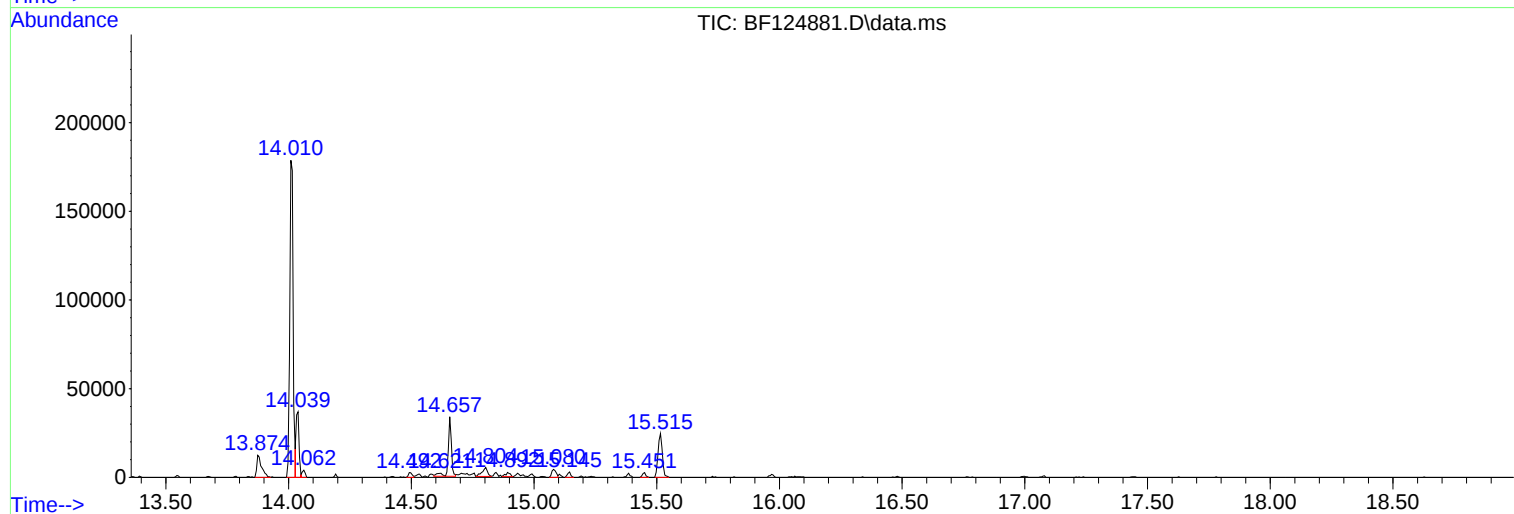
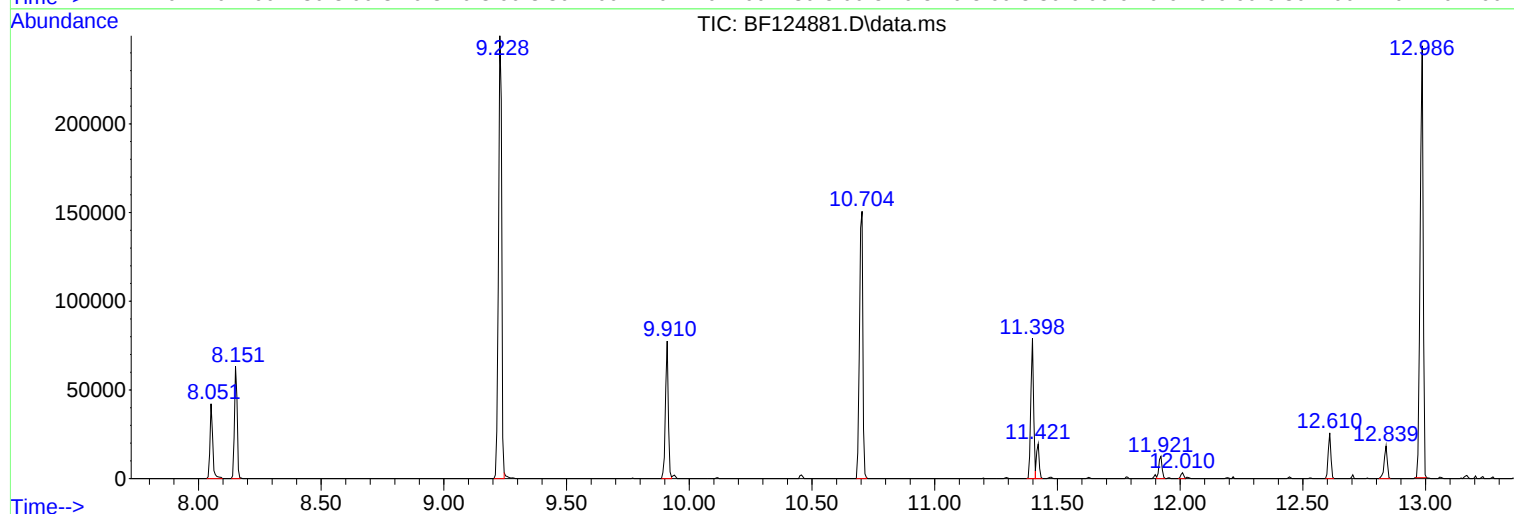
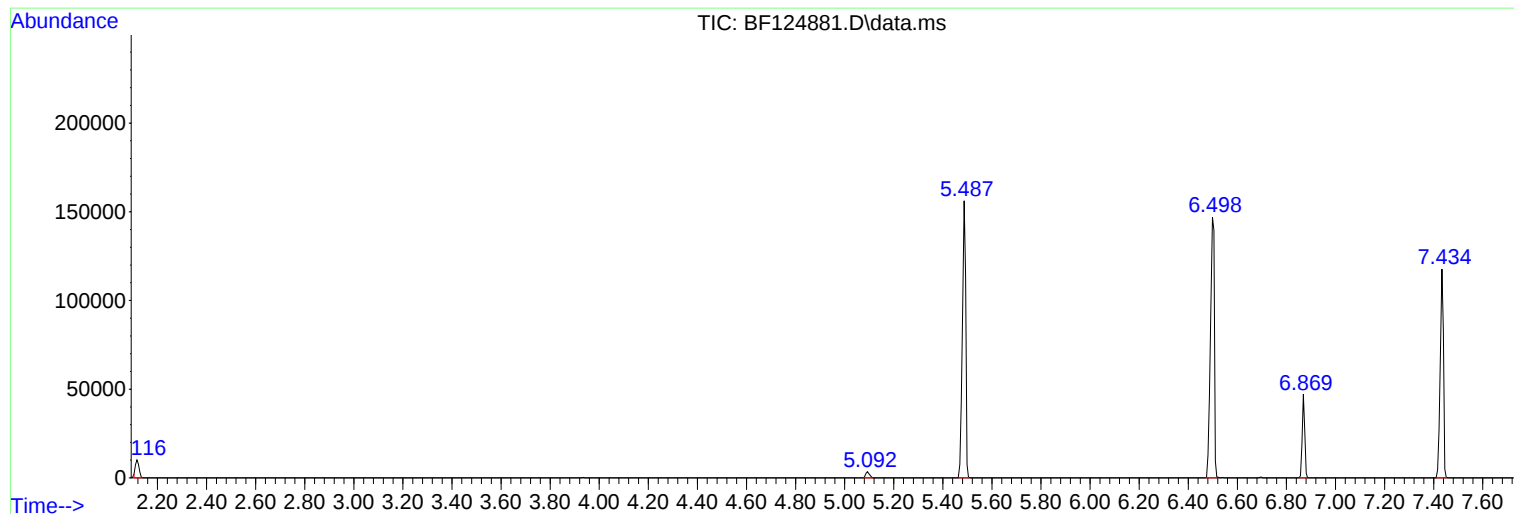
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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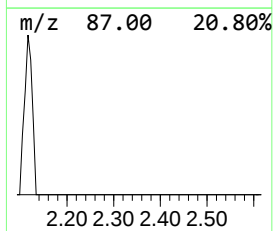
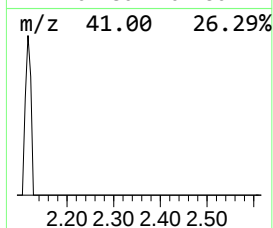
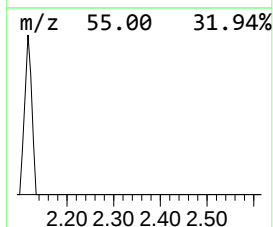
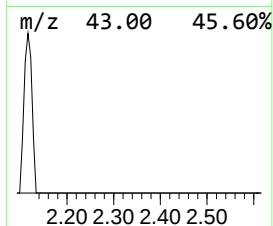
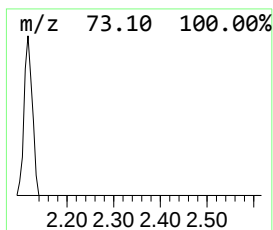
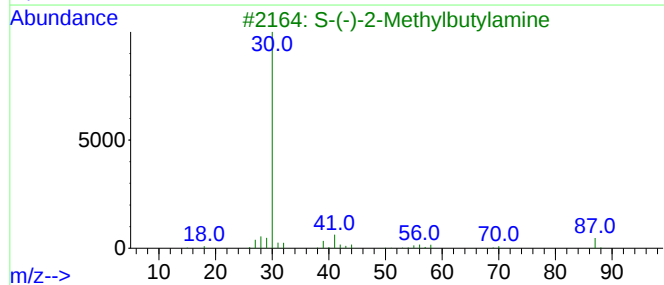
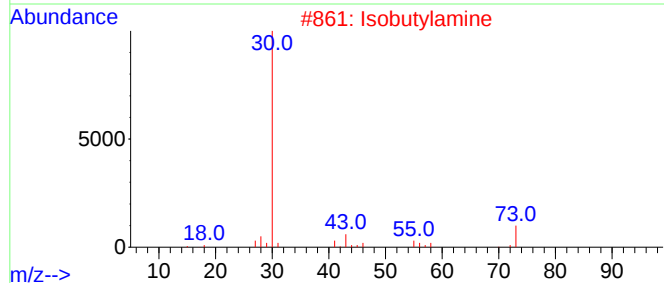
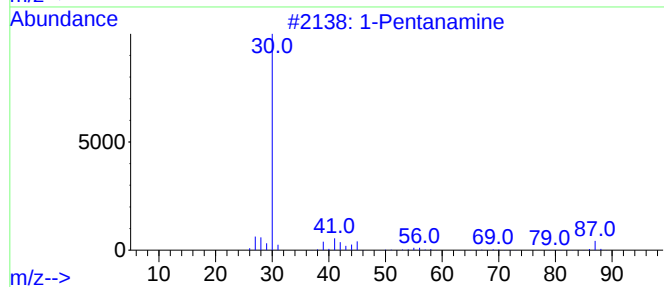
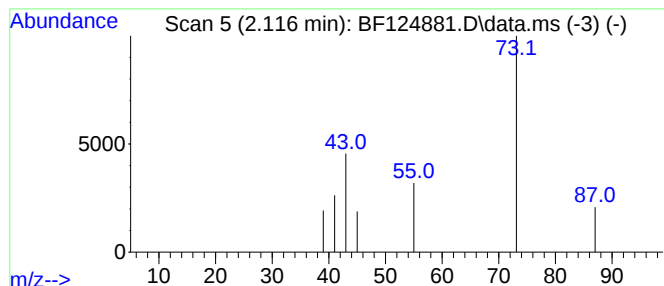
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.116 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	6.10 ng	10304	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanamine	87	C5H13N	000110-58-7	7
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	4
4			1-Butanamine	73	C4H11N	000109-73-9	3
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	3



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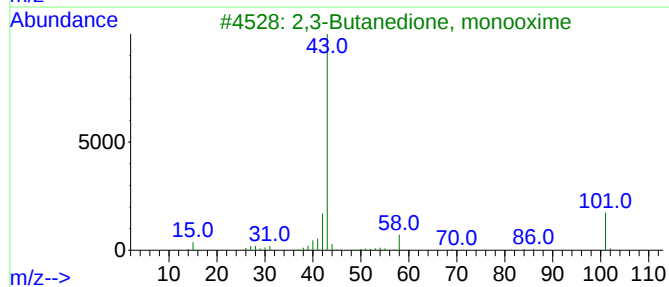
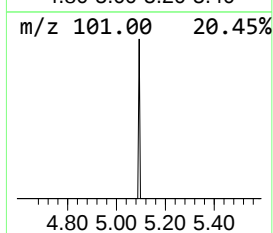
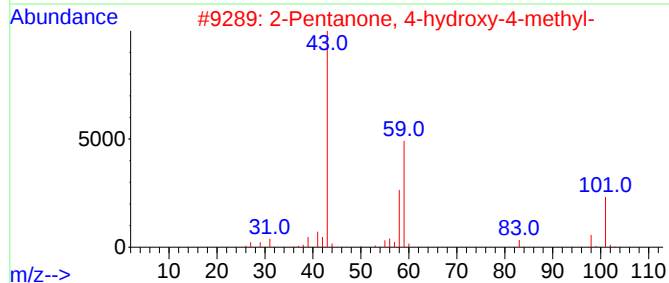
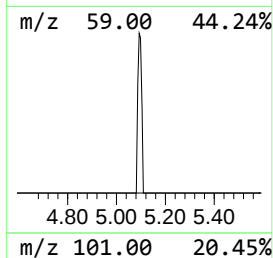
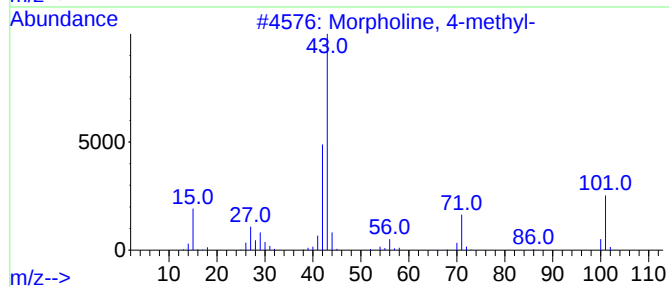
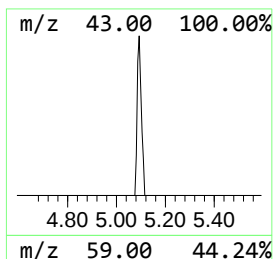
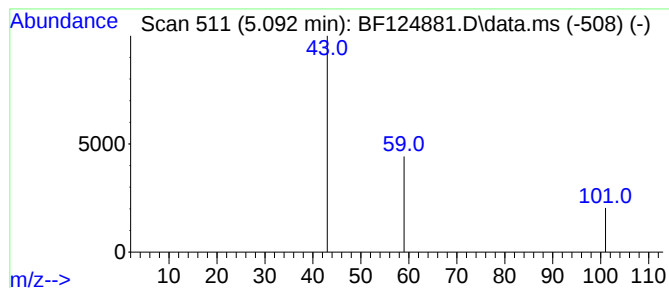
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.092 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	2.27 ng	3838	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	4
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	4
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	3
4			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	3
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	2



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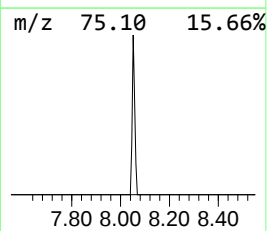
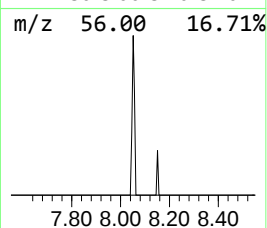
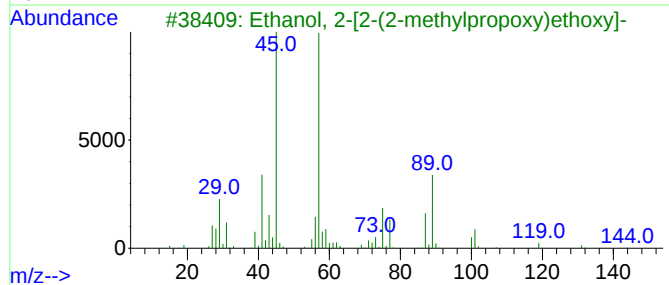
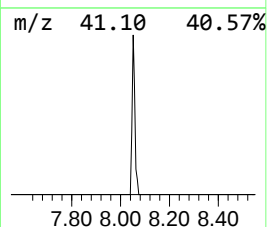
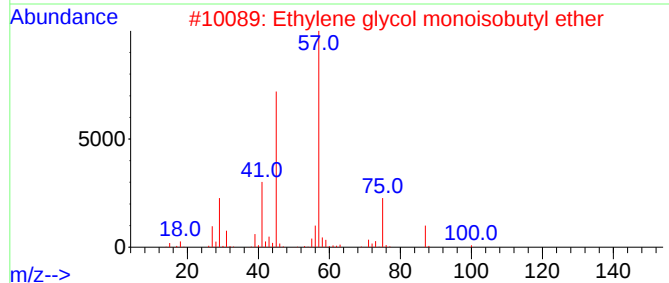
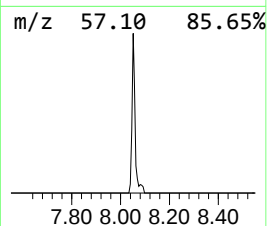
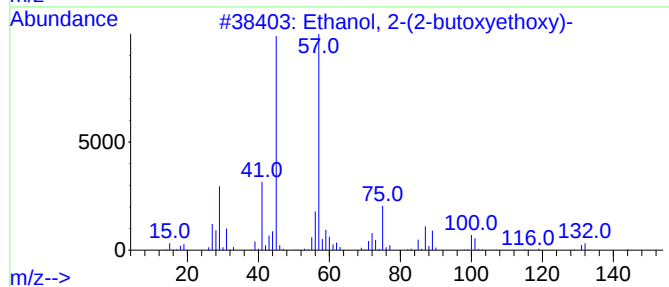
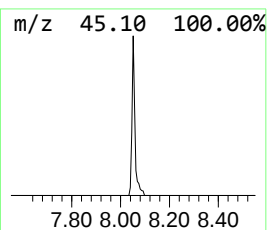
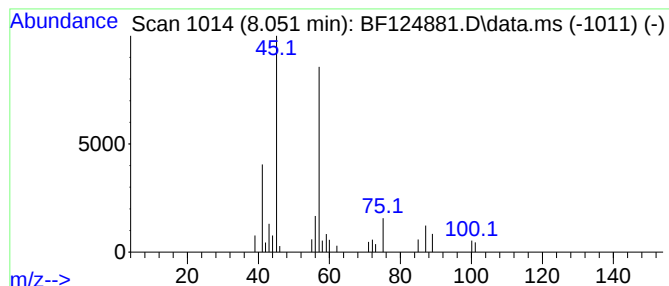
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	13.42 ng	32819	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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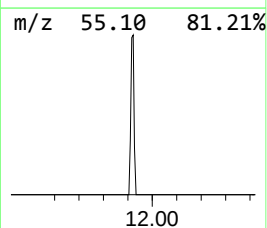
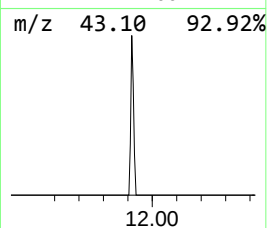
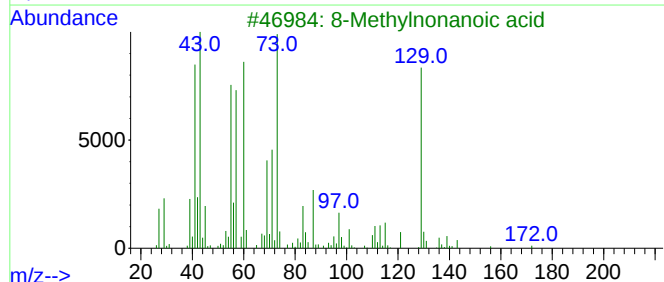
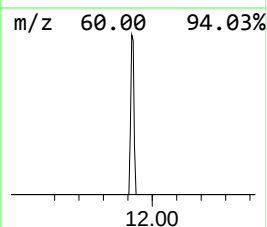
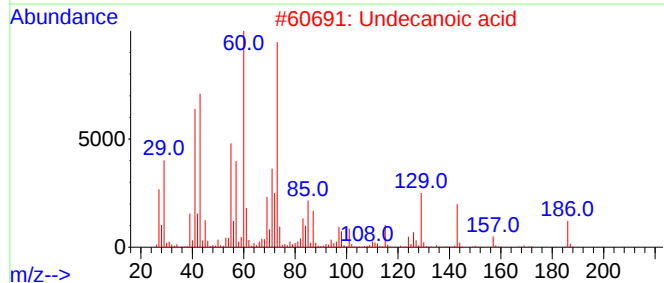
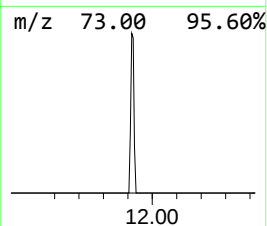
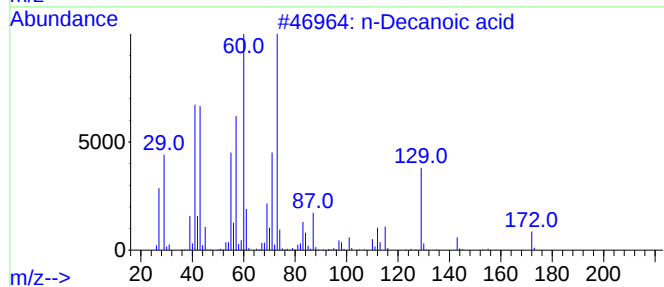
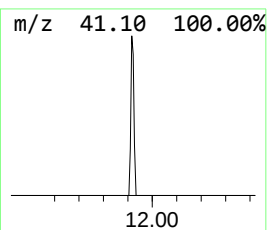
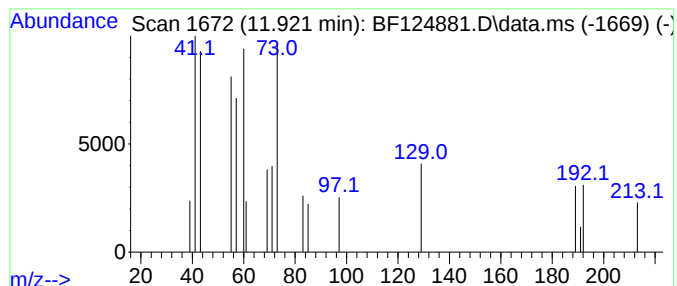
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Peak Number 4 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.57 ng	11267	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	50
2			Undecanoic acid	186	C11H22O2	000112-37-8	40
3			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38
4			Dodecanoic acid	200	C12H24O2	000143-07-7	36
5			Lactose	342	C12H22O11	000063-42-3	28



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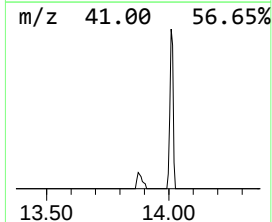
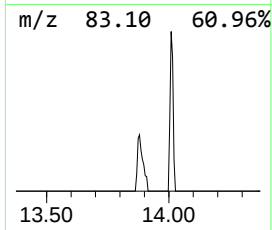
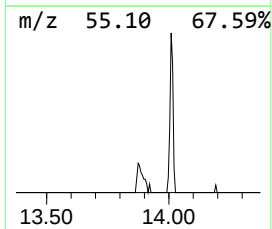
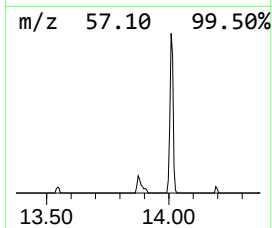
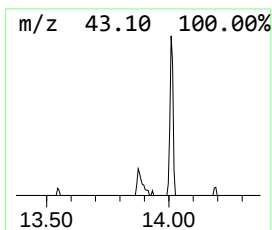
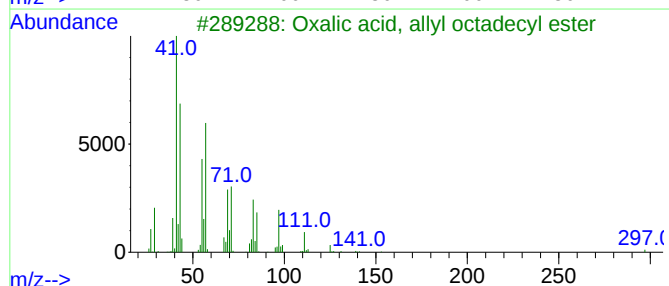
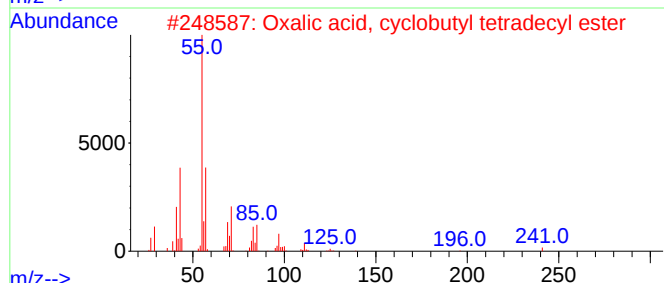
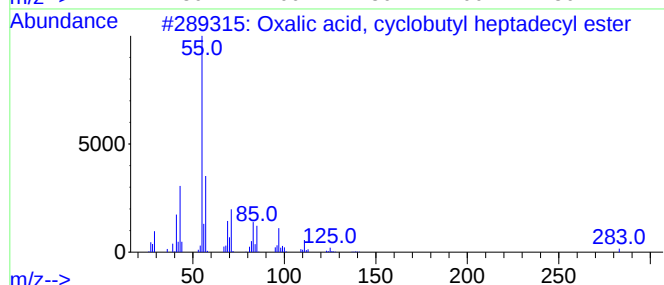
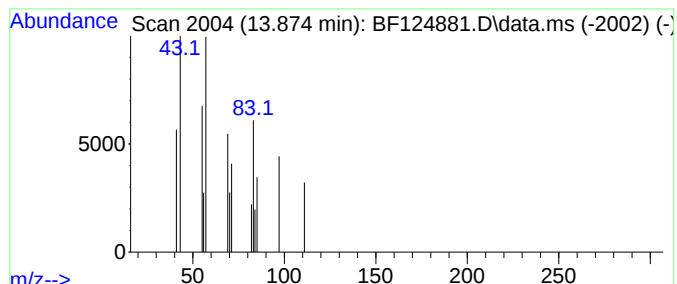
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Peak Number 5 Oxalic acid, cyclobutyl hep... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	11.33 ng	17056	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	53
2			Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	45
3			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	45
4			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	40
5			Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	37



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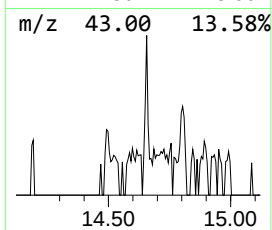
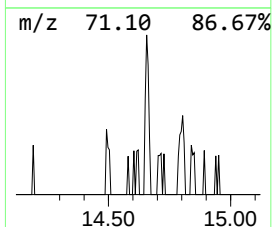
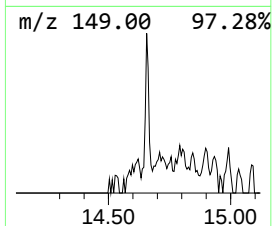
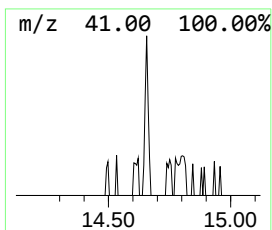
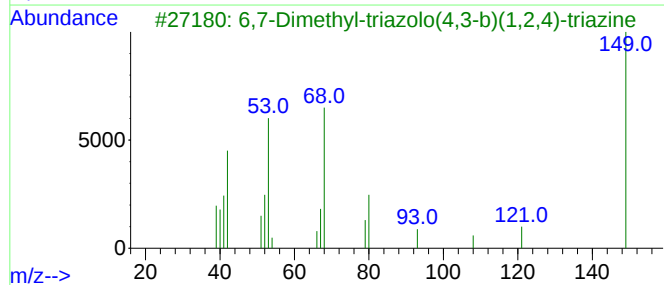
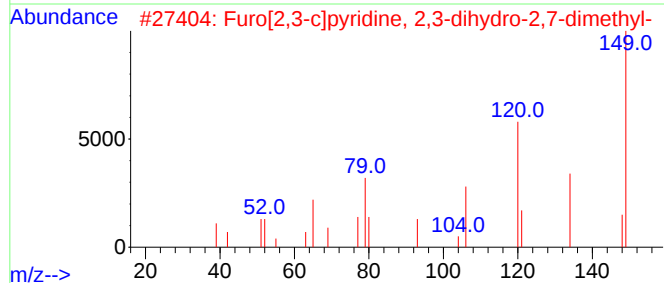
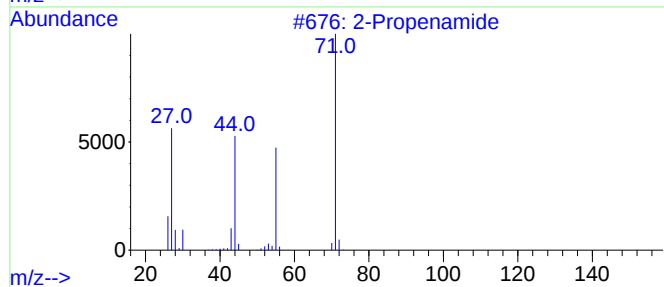
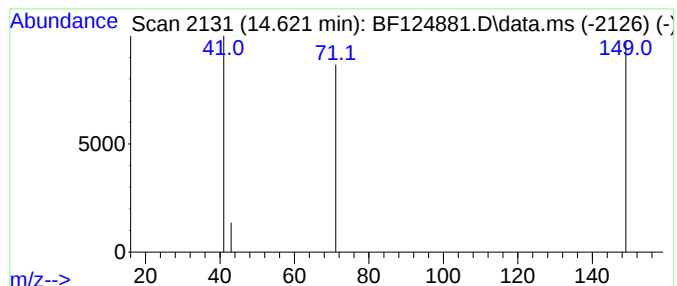
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.621 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	2.04 ng	3077	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenamide		71	C3H5NO		000079-06-1	3
2	Furo[2,3-c]pyridine, 2,3-dihydro...		149	C9H11NO		069022-82-8	2
3	6,7-Dimethyl-triazolo(4,3-b)(1,2...		149	C6H7N5		061139-73-9	2
4	2-Ethylformanilide		149	C9H11NO		002860-30-2	2
5	3(2H)-Thiophenone, dihydro-, oxi...		149	C4H7NO3S		1010327-57-0	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124881.D
Acq On : 30 Jul 2021 17:52
Operator : JU/CG
Sample : M3238-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

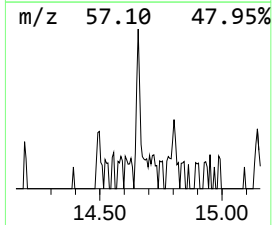
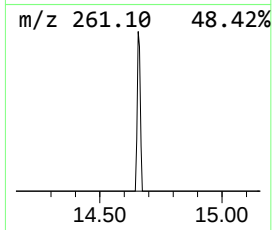
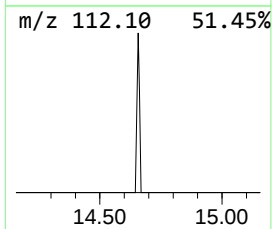
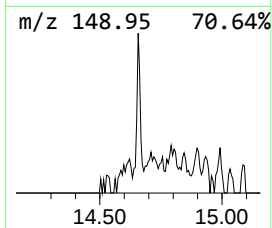
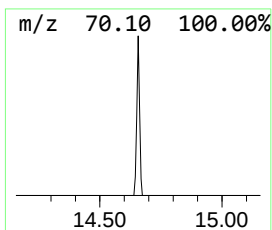
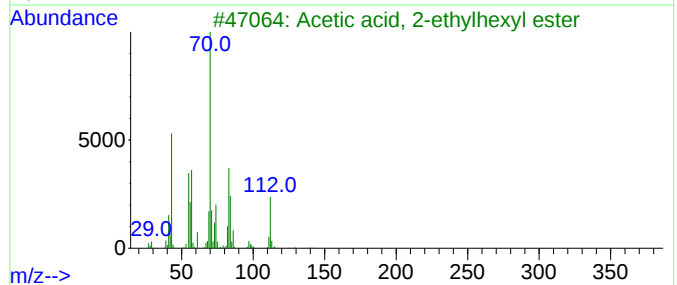
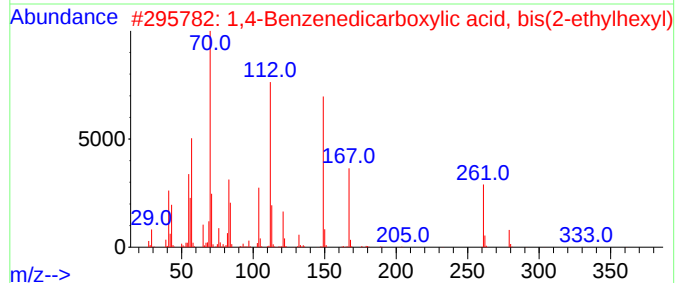
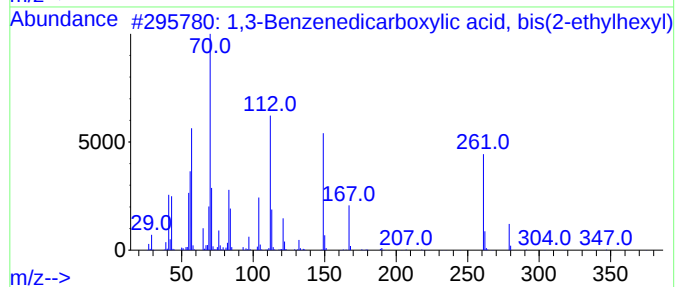
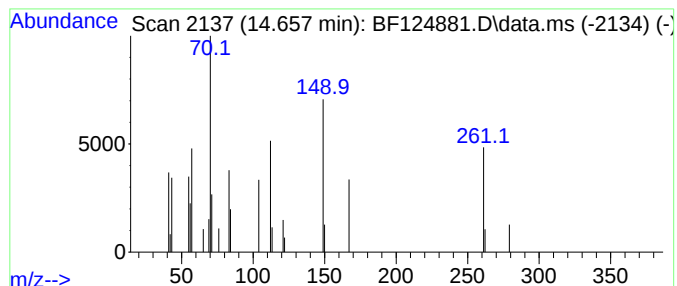
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,3-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.657	18.35 ng	27615	Chrysene-d12	14.039	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	72
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
3	Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	35
4	Carbonic acid, 2-chloroethyl 2-e...	236	C11H21ClO3	1000357-88-2	27
5	Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124881.D
Acq On : 30 Jul 2021 17:52
Operator : JU/CG
Sample : M3238-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
221

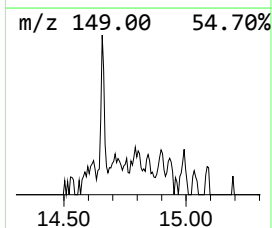
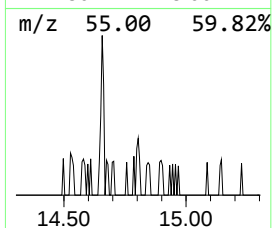
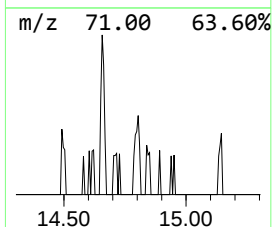
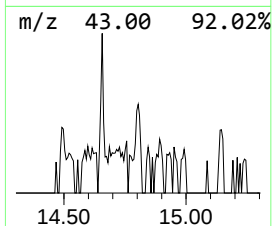
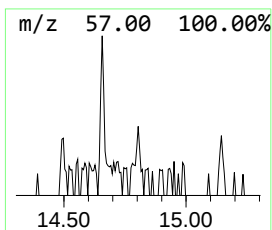
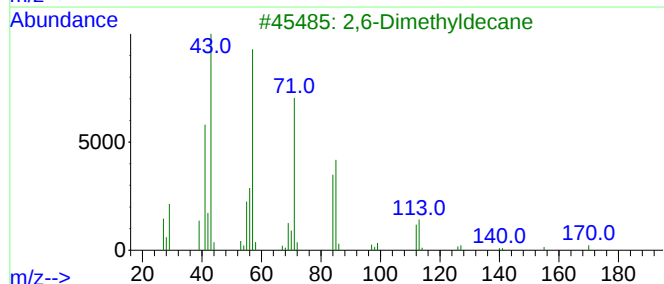
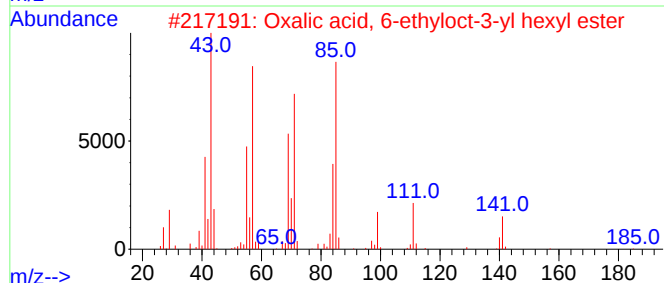
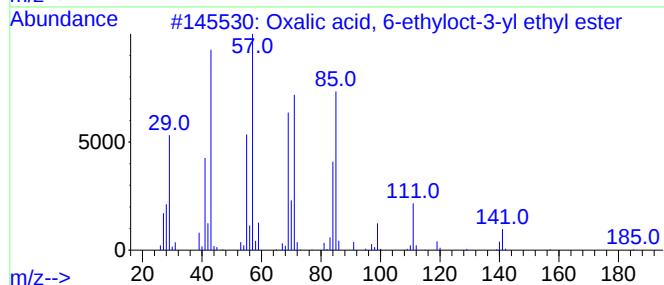
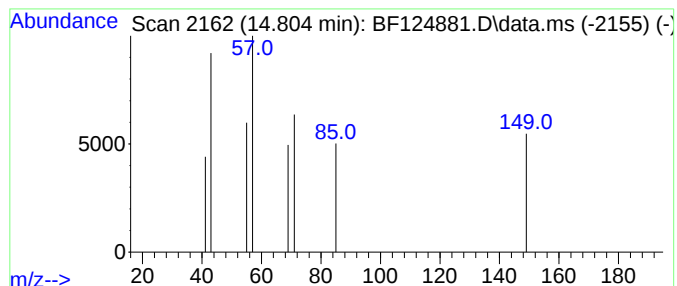
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.804 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	5.17 ng	7754	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, 6-ethyloct-3-yl eth...	258	C14H26O4	1000309-33-9	42
2			Oxalic acid, 6-ethyloct-3-yl hex...	314	C18H34O4	1000309-34-4	42
3			2,6-Dimethyldecane	170	C12H26	013150-81-7	9
4			Undecane, 3,7-dimethyl-	184	C13H28	017301-29-0	9
5			Octacosane	394	C28H58	000630-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124881.D
Acq On : 30 Jul 2021 17:52
Operator : JU/CG
Sample : M3238-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
221

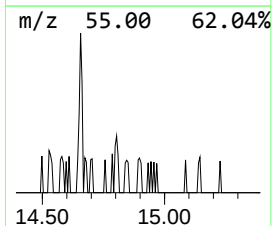
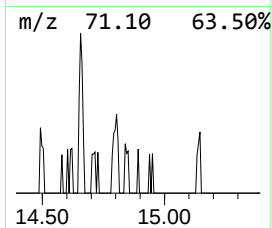
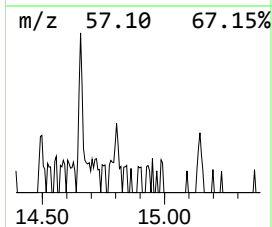
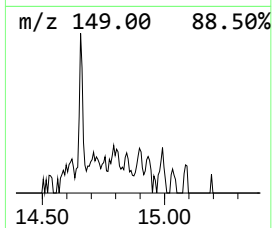
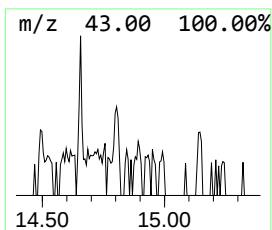
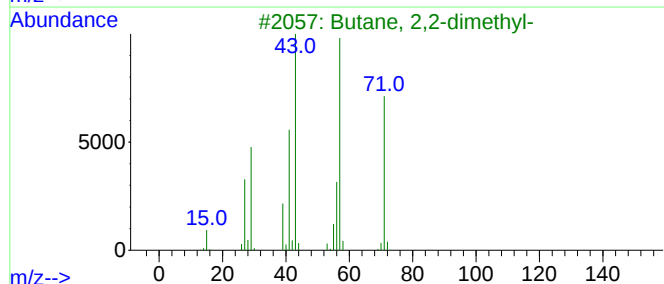
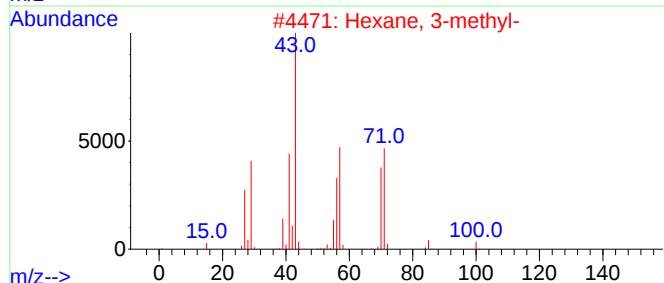
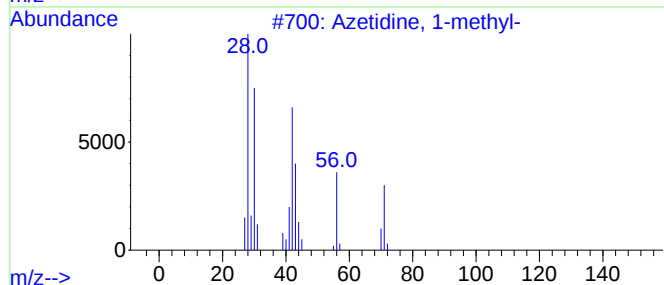
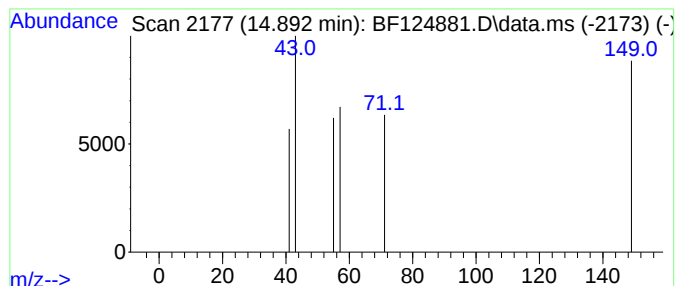
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.892 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.892	2.08 ng	3124	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	4
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	4
4			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3
5			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF073021\
Data File : BF124881.D
Acq On : 30 Jul 2021 17:52
Operator : JU/CG
Sample : M3238-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown5.092	5.092	2.3	ng	3838	1	6.869	33772	20.0
Ethanol, 2-(2-b...	8.051	13.4	ng	32819	2	8.151	48909	20.0
n-Decanoic acid	11.922	3.6	ng	11267	4	11.398	63207	20.0
Oxalic acid, cy...	13.874	11.3	ng	17056	5	14.039	30105	20.0
unknown14.621	14.621	2.0	ng	3077	5	14.039	30105	20.0
1,3-Benzenedica...	14.657	18.4	ng	27615	5	14.039	30105	20.0
unknown14.804	14.804	5.2	ng	7754	6	15.515	30002	20.0
unknown14.892	14.892	2.1	ng	3124	6	15.515	30002	20.0