

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
 Data File : BF124810.D
 Acq On : 28 Jul 2021 00:19
 Operator : JU/CG
 Sample : M3171-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-078

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: BF124810.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	4	8	11	rBB	8279	8991	4.98%	0.660%
2	5.487	573	578	581	rBB	145401	131549	72.91%	9.657%
3	6.492	745	749	752	rBV	126821	137740	76.34%	10.112%
4	6.869	810	813	816	rBB	48425	33263	18.44%	2.442%
5	7.434	904	909	912	rBB	111908	91419	50.67%	6.711%
6	8.051	1011	1014	1019	rBB	21229	14928	8.27%	1.096%
7	8.151	1028	1031	1034	rBB	59877	46061	25.53%	3.381%
8	9.228	1210	1214	1217	rBV	220716	180433	100.00%	13.246%
9	9.910	1327	1330	1333	rBV	72715	55856	30.96%	4.100%
10	10.698	1460	1464	1467	rBB	135467	111344	61.71%	8.174%
11	11.392	1579	1582	1585	rBV	66373	55504	30.76%	4.075%
12	11.916	1668	1671	1674	rBB	15711	10432	5.78%	0.766%
13	12.604	1786	1788	1790	rBB	3050	2174	1.20%	0.160%
14	12.833	1825	1827	1829	rBV	4042	2748	1.52%	0.202%
15	12.980	1848	1852	1855	rBV	181665	152724	84.64%	11.212%
16	13.204	1887	1890	1895	rBB	6257	5184	2.87%	0.381%
17	13.545	1945	1948	1953	rBB	9421	8515	4.72%	0.625%
18	13.880	2001	2005	2014	rVB2	18783	26087	14.46%	1.915%
19	14.033	2027	2031	2034	rBV	38381	31136	17.26%	2.286%
20	14.192	2054	2058	2061	rBV	17560	14325	7.94%	1.052%
21	14.498	2107	2110	2112	rBV	20859	17630	9.77%	1.294%
22	14.527	2112	2115	2123	rVB2	4985	9041	5.01%	0.664%
23	14.804	2159	2162	2166	rVB	13693	14565	8.07%	1.069%
24	14.880	2172	2175	2179	rBB	4653	5522	3.06%	0.405%
25	14.957	2183	2188	2191	rBB2	2525	2764	1.53%	0.203%
26	15.145	2216	2220	2225	rVB	20687	22597	12.52%	1.659%
27	15.198	2225	2229	2232	rBV2	2225	3569	1.98%	0.262%
28	15.510	2278	2282	2289	rBB2	30461	45637	25.29%	3.350%
29	15.733	2315	2320	2325	rBB2	2858	4058	2.25%	0.298%
30	15.974	2355	2361	2367	rBB2	10650	15822	8.77%	1.162%
31	16.039	2367	2372	2382	rBV3	5728	16536	9.16%	1.214%
32	16.251	2404	2408	2414	rVB	2064	3651	2.02%	0.268%
33	16.486	2442	2448	2453	rBV	6239	9479	5.25%	0.696%
34	16.786	2491	2499	2503	rBB2	2786	5421	3.00%	0.398%
35	17.086	2543	2550	2557	rVB3	4002	8058	4.47%	0.592%
36	17.609	2630	2639	2646	rBV5	10443	28531	15.81%	2.094%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.656	2646	2647	2655	rVB3	3271	4582	2.54%	0.336%
38	17.798	2669	2671	2676	rVB2	3656	5506	3.05%	0.404%
39	18.162	2729	2733	2739	rBB3	3357	6232	3.45%	0.457%
40	18.615	2806	2810	2819	rVB4	5383	12574	6.97%	0.923%

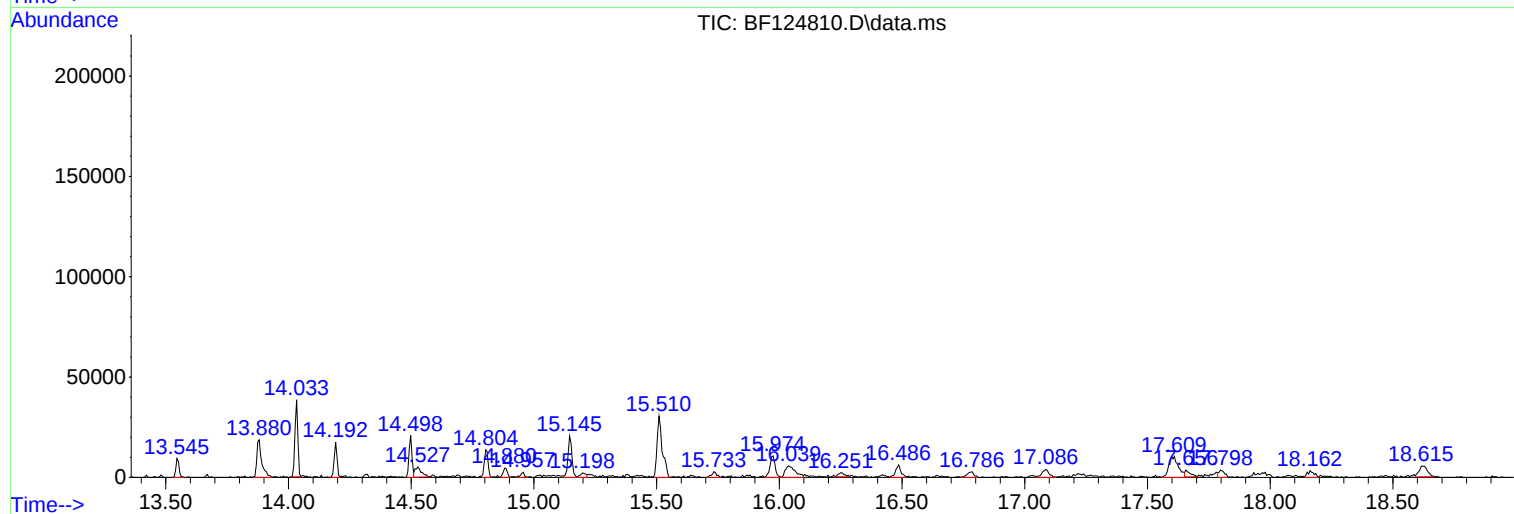
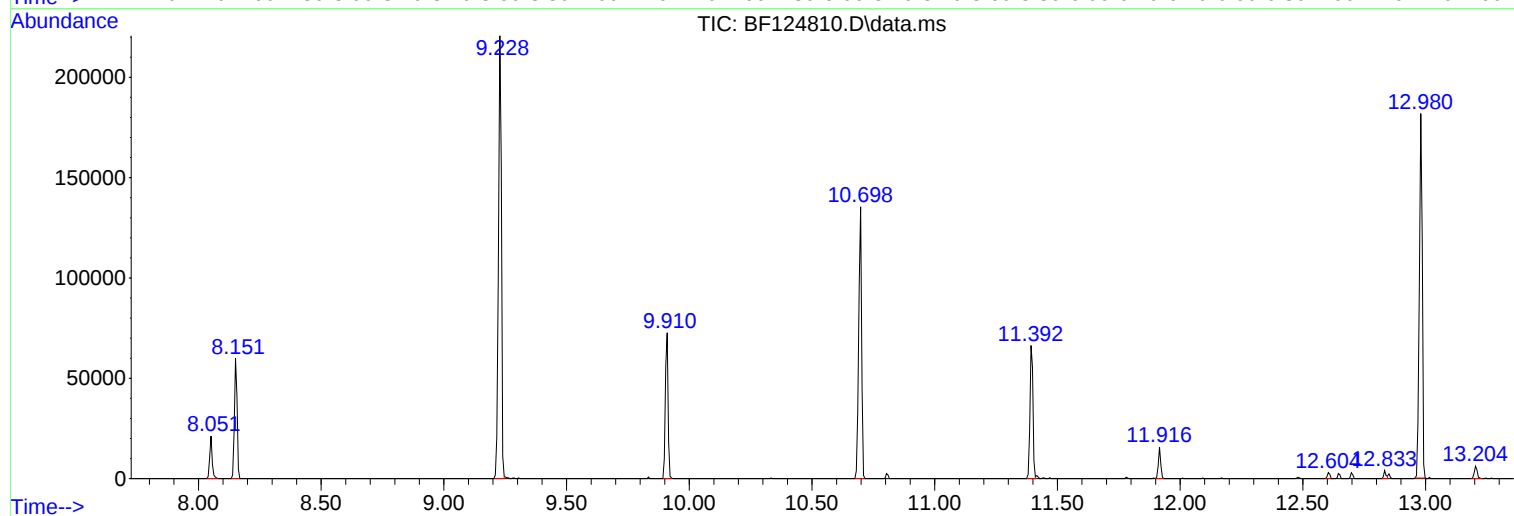
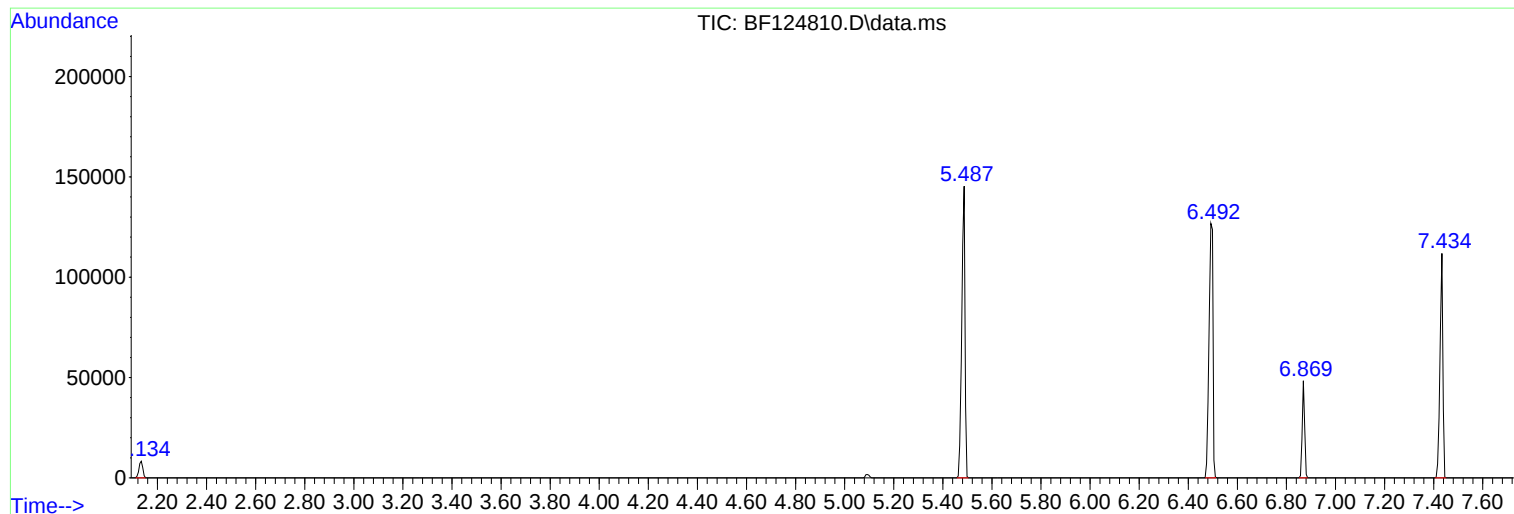
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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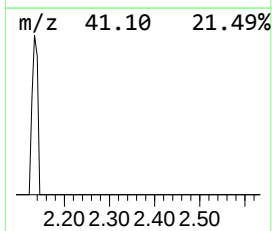
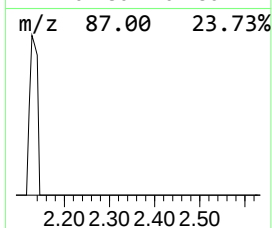
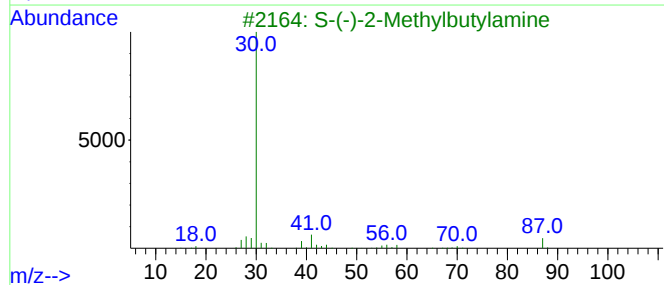
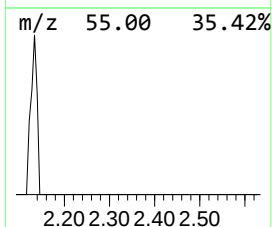
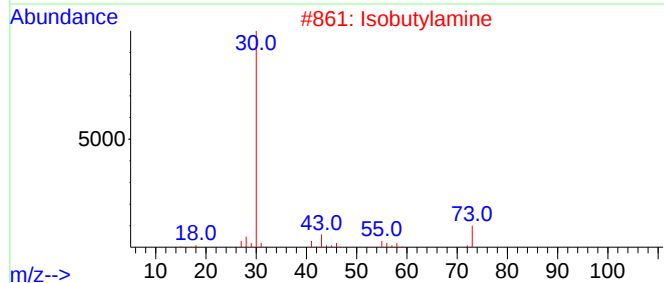
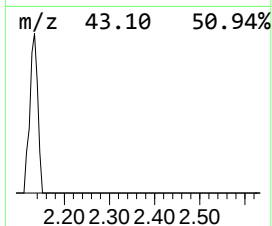
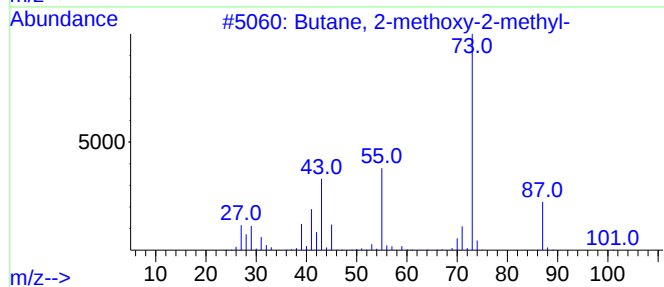
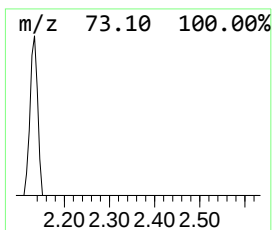
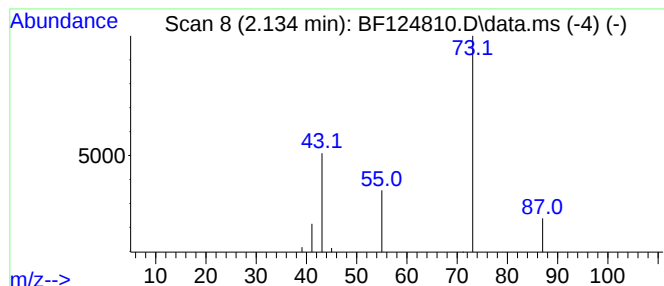
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	5.41 ng	8991	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	64
2			Isobutylamine	73	C4H11N	000078-81-9	5
3			S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	4
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5			3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4



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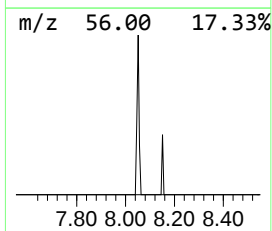
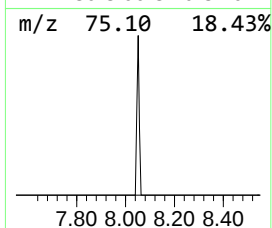
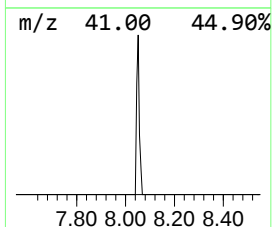
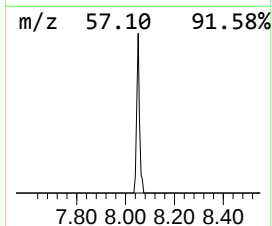
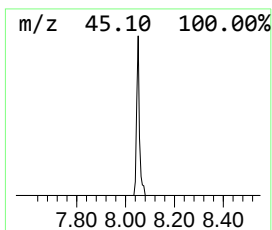
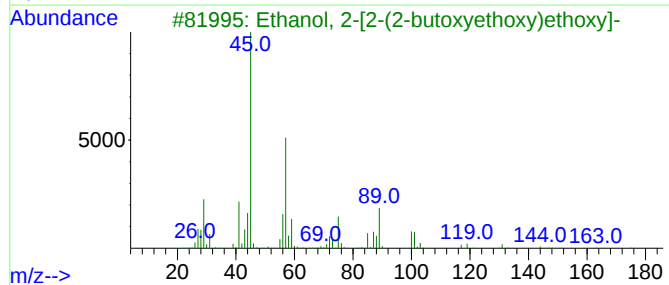
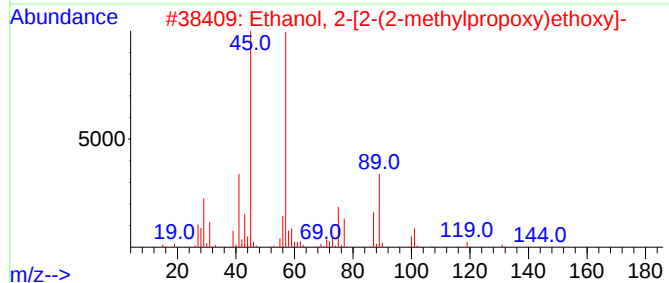
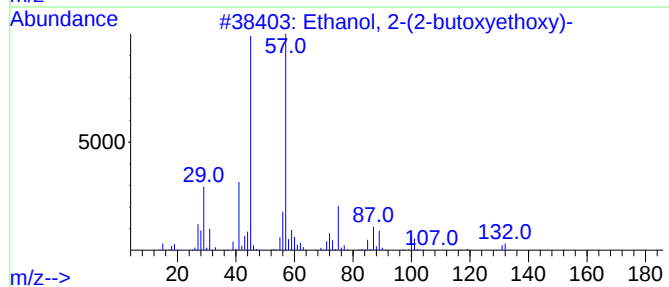
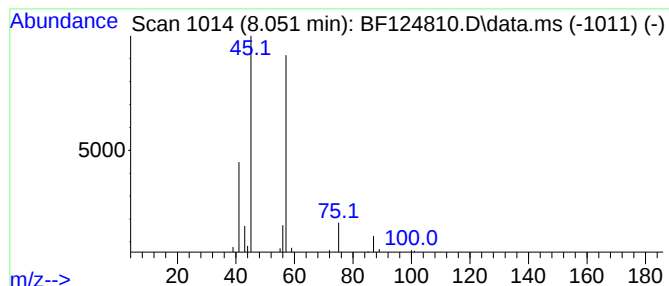
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	6.48 ng	14928	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
4			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	39
5			Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	10



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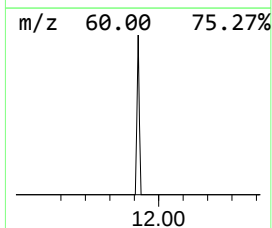
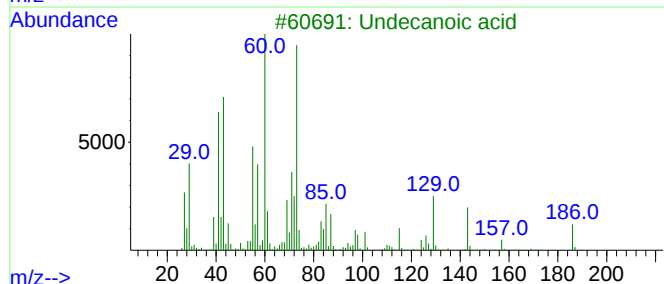
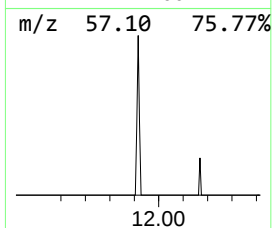
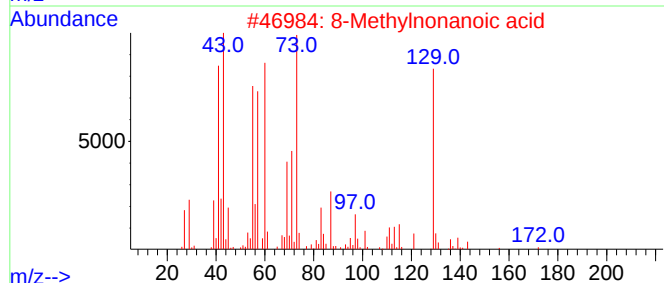
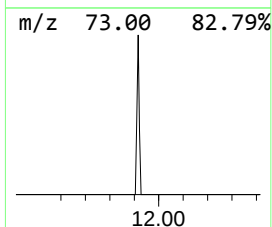
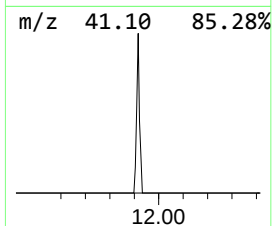
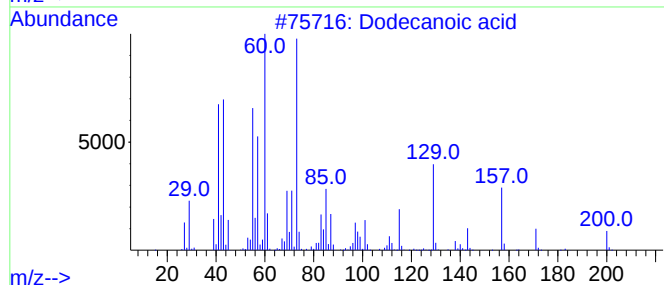
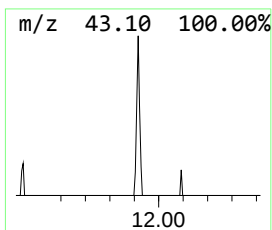
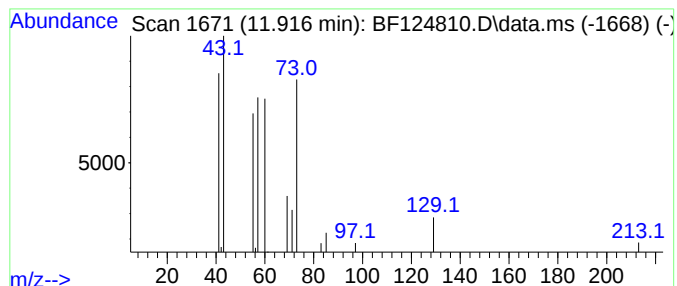
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Dodecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.916	3.76 ng	10432	Phenanthrene-d10	11.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	64
2	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Butanoic acid, 3-methyl-, 1-meth...	144	C8H16O2	032665-23-9	37



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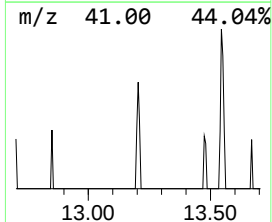
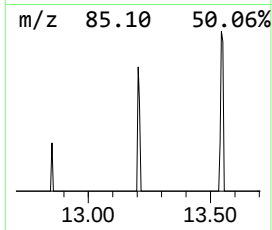
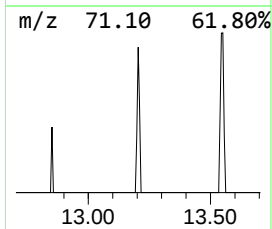
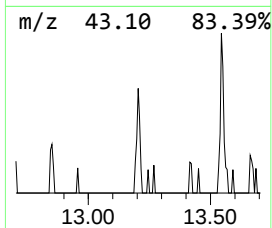
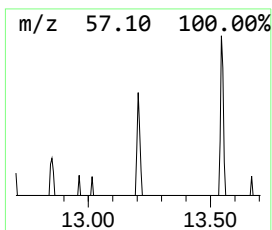
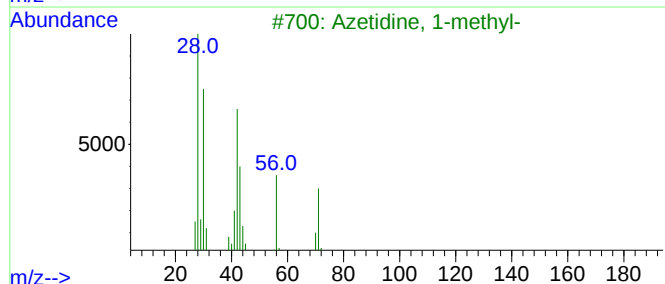
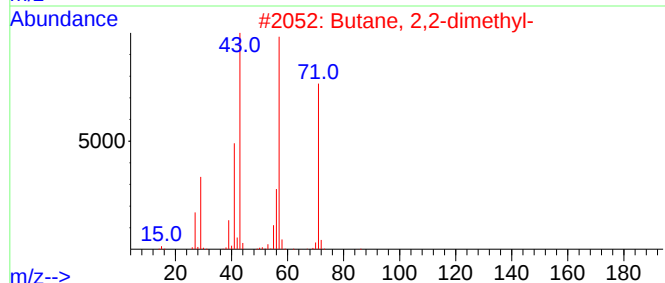
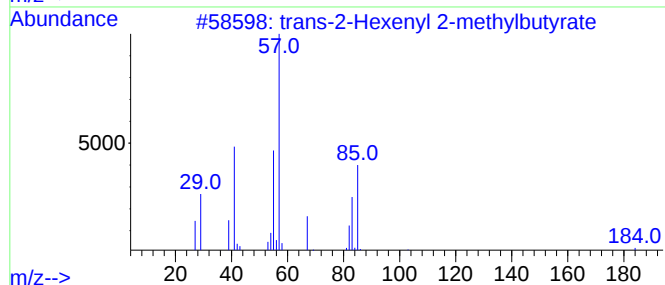
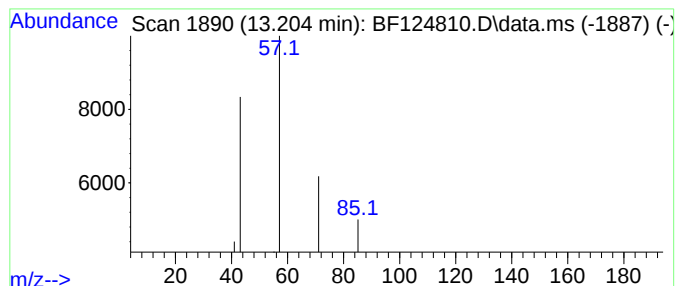
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown13.204 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.204	3.33 ng	5184	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
2			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
3			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
4			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
5			Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4



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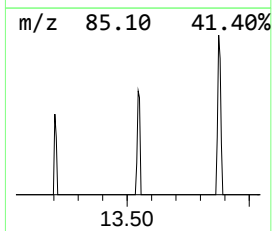
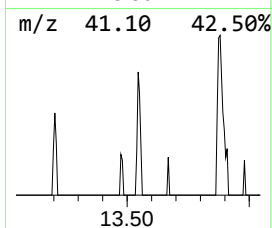
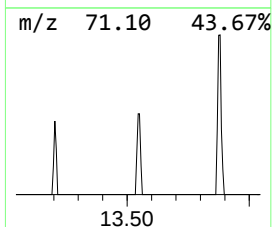
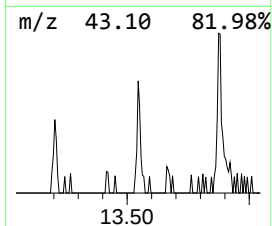
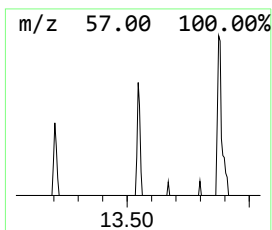
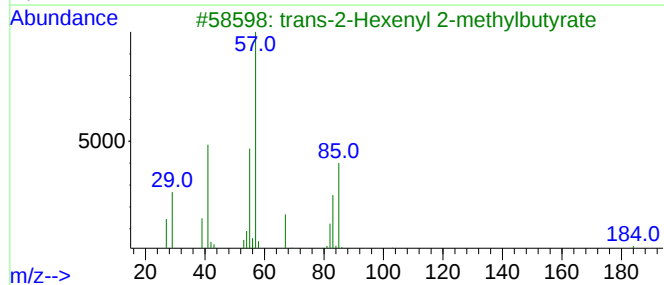
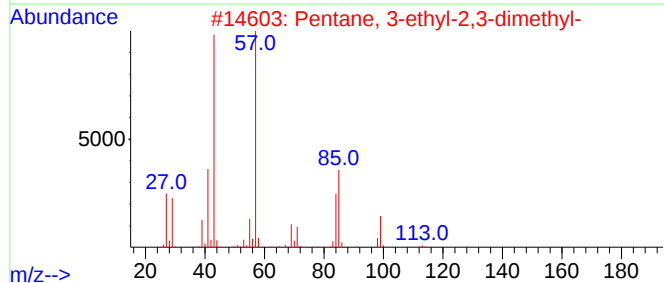
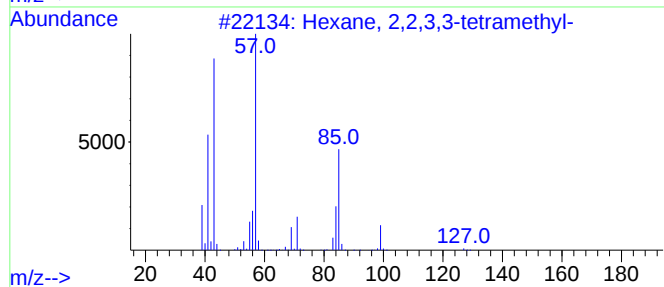
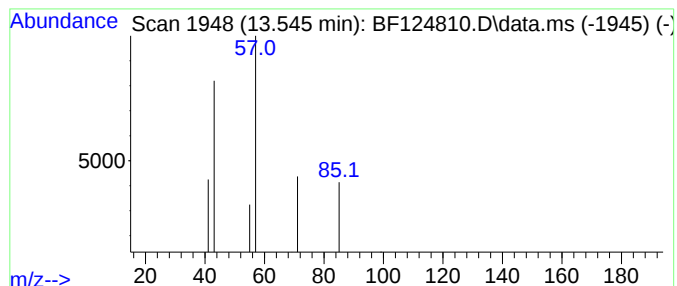
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.545 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.545	5.47 ng	8515	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	45
2			Pentane, 3-ethyl-2,3-dimethyl-	128	C9H20	016747-33-4	38
3			trans-2-Hexenyl 2-methylbutyrate	184	C11H20O2	1000433-23-8	9
4			Ether, heptyl hexyl	200	C13H28O	007289-40-9	9
5			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

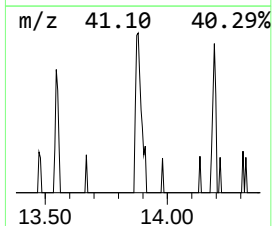
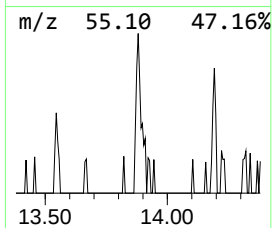
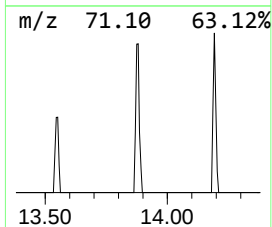
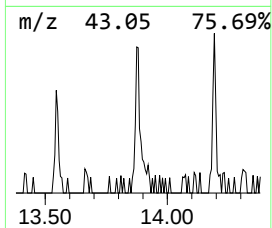
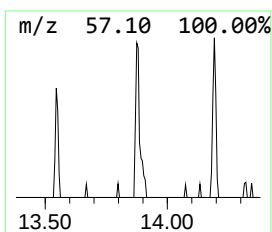
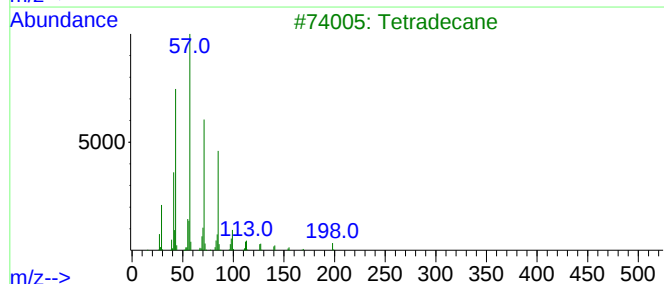
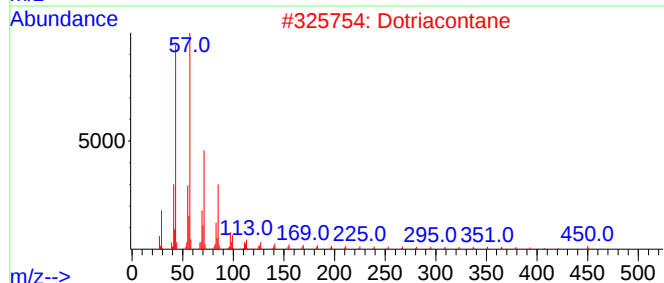
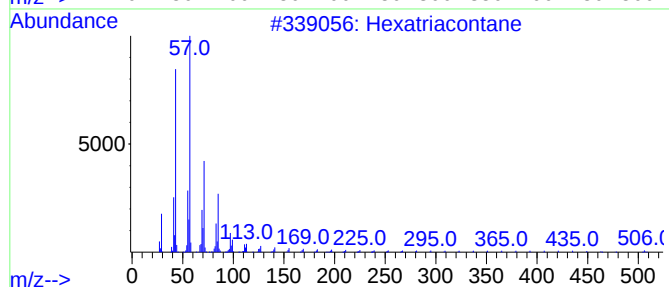
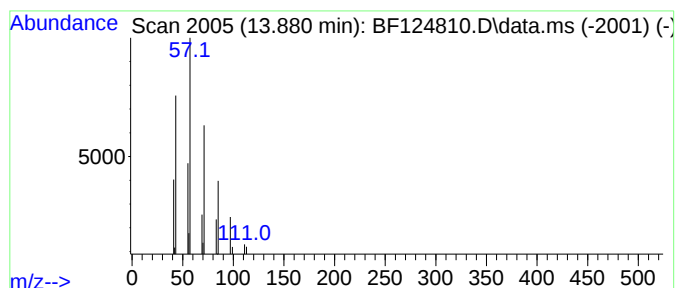
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexatriacontane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.880	16.76 ng	26087	Chrysene-d12	14.033	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	83
2	Dotriacontane	451	C32H66	000544-85-4	78
3	Tetradecane	198	C14H30	000629-59-4	53
4	Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	53
5	Tridecane	184	C13H28	000629-50-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-078

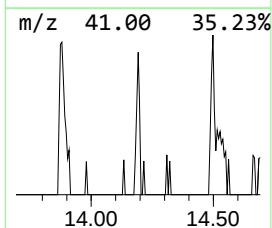
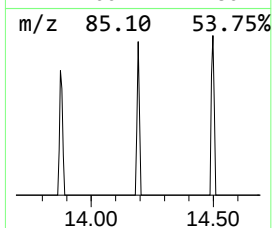
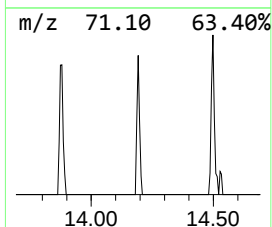
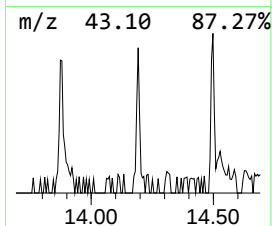
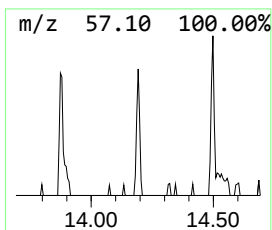
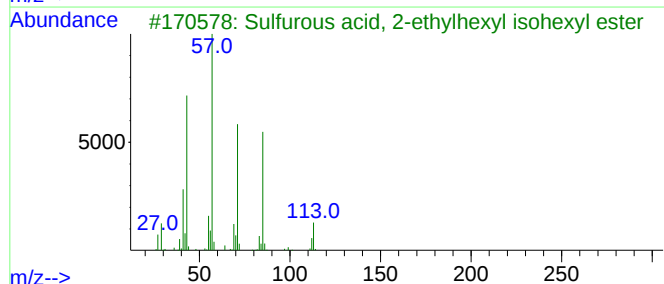
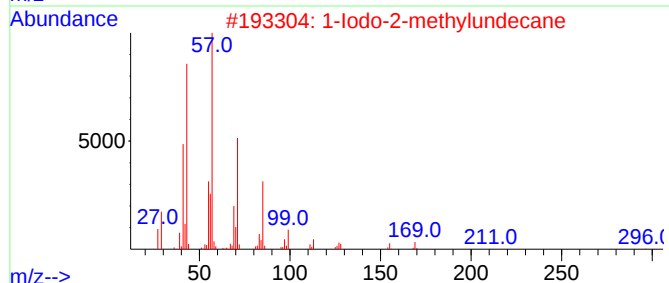
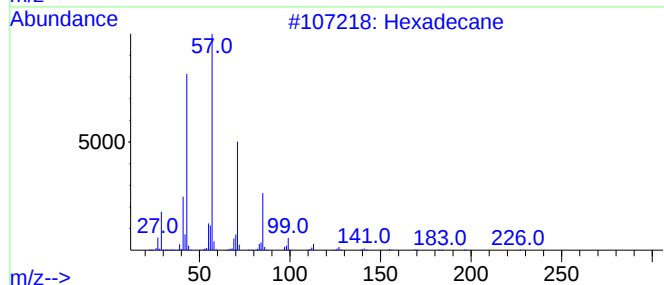
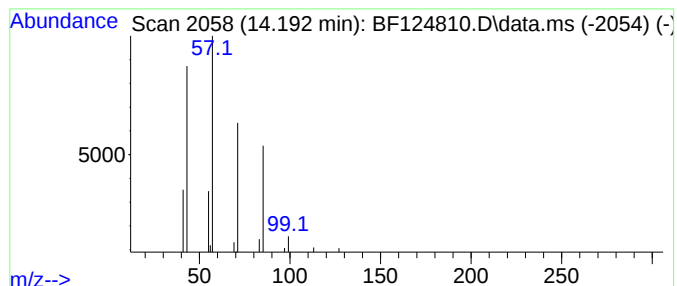
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	9.20 ng	14325	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	78
2			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	72
3			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64
4			Nonadecane	268	C19H40	000629-92-5	59
5			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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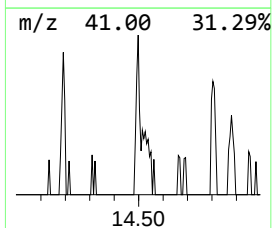
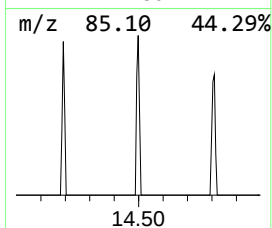
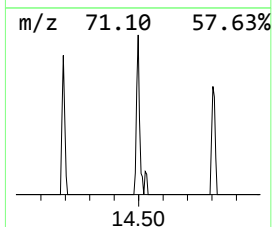
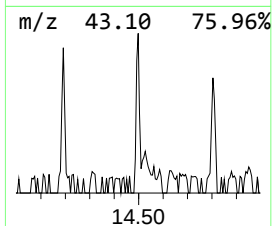
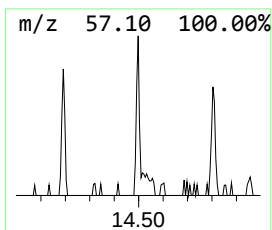
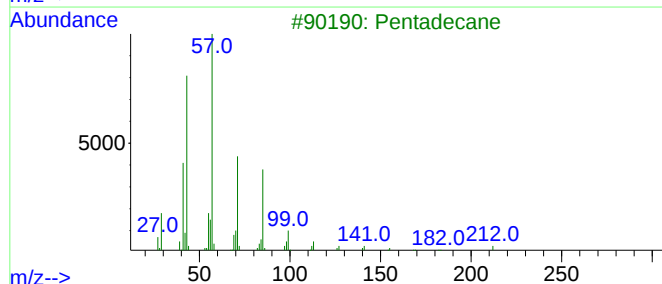
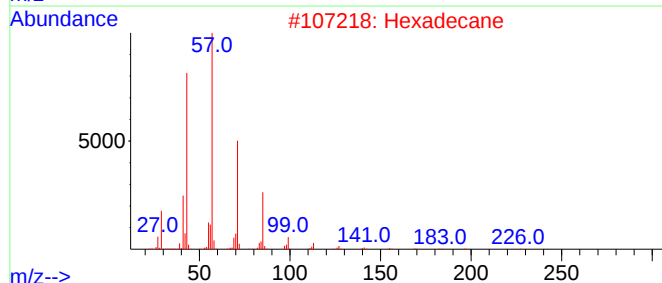
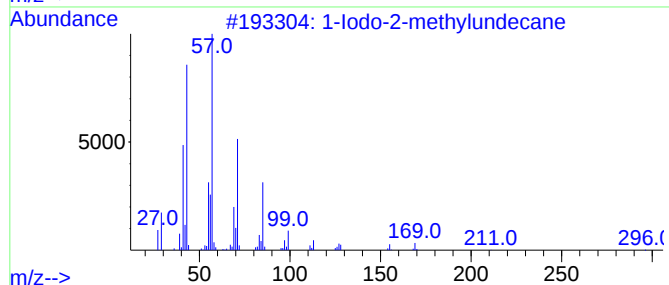
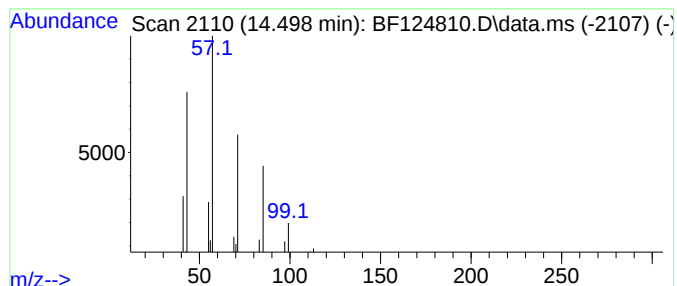
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Iodo-2-methylundecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	11.32 ng	17630	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59
2			Hexadecane	226	C16H34	000544-76-3	59
3			Pentadecane	212	C15H32	000629-62-9	53
4			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	53
5			Tridecane	184	C13H28	000629-50-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-078

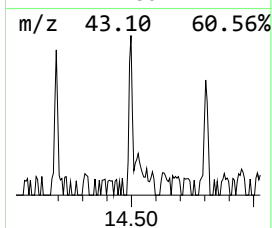
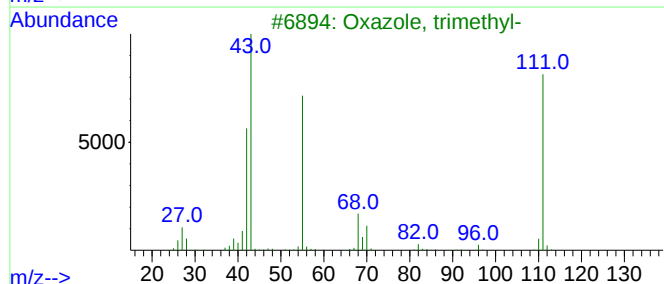
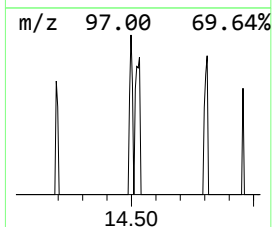
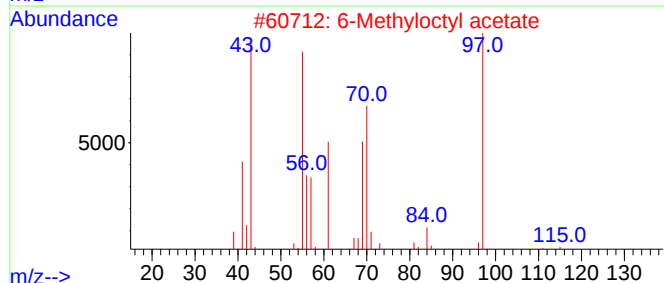
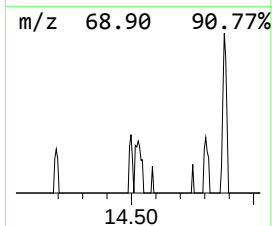
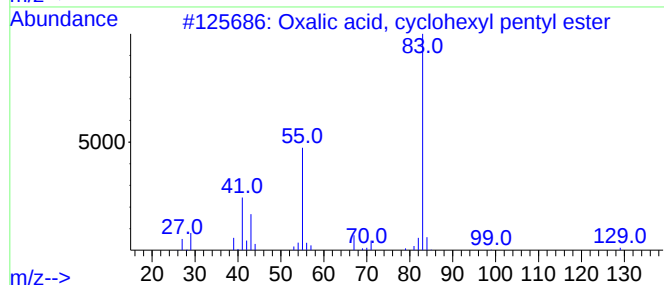
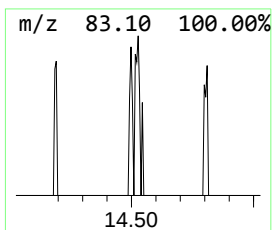
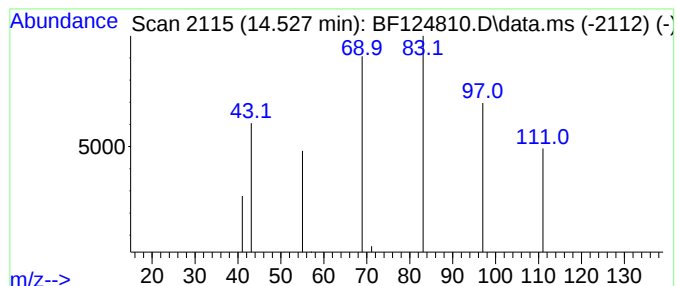
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.527 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	5.81 ng	9041	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclohexyl pentyl e...	242	C13H22O4	1000309-30-6	9
2			6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	9
3			Oxazole, trimethyl-	111	C6H9NO	020662-84-4	7
4			Oxazole, 4,5-dimethyl-	97	C5H7NO	020662-83-3	7
5			2-Acetyl-1-pyrroline	111	C6H9NO	085213-22-5	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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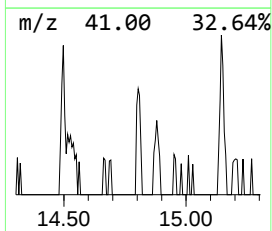
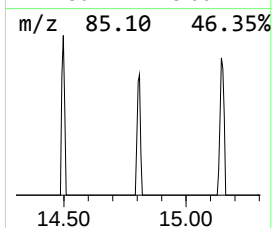
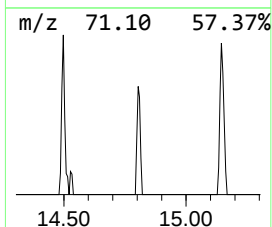
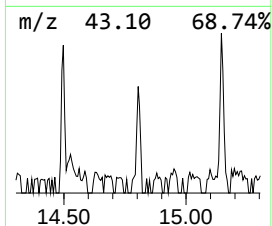
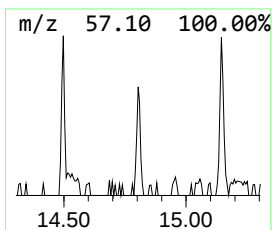
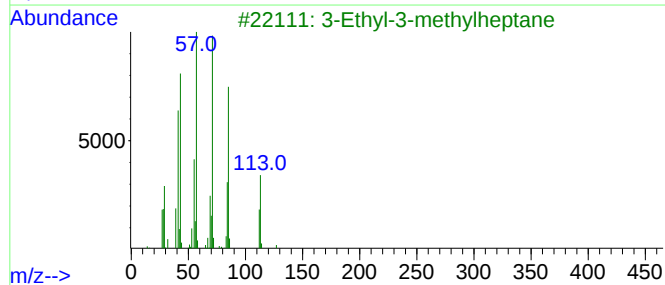
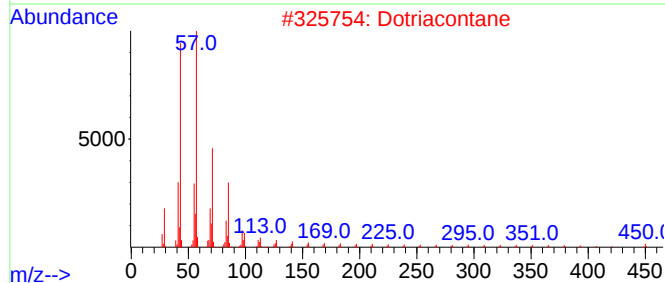
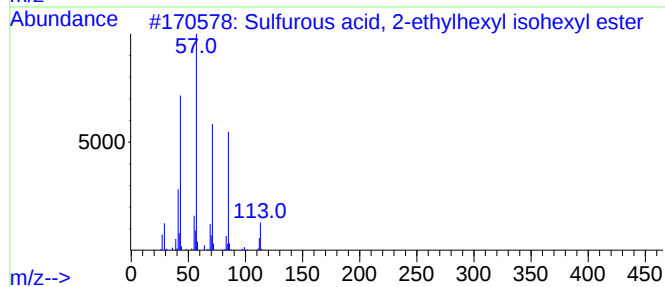
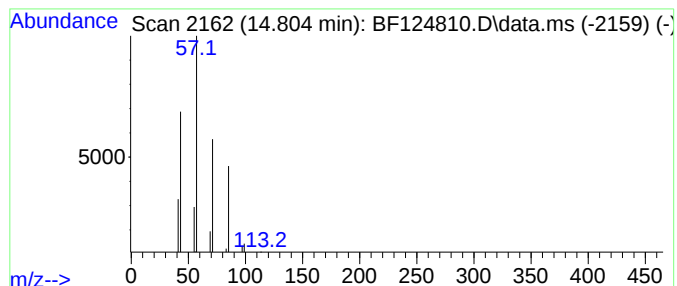
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Sulfurous acid, 2-ethylhexy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	6.38 ng	14565	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
2			Dotriacontane	451	C32H66	000544-85-4	72
3			3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	64
4			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64
5			Tetradecane	198	C14H30	000629-59-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
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Misc :
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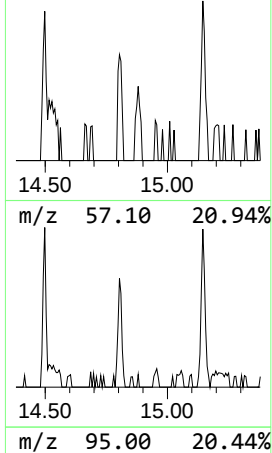
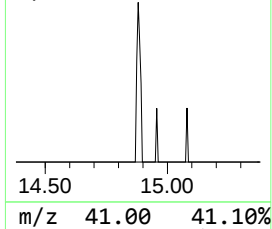
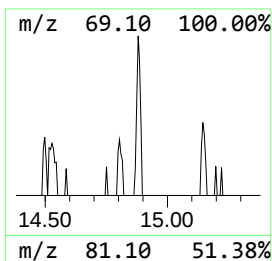
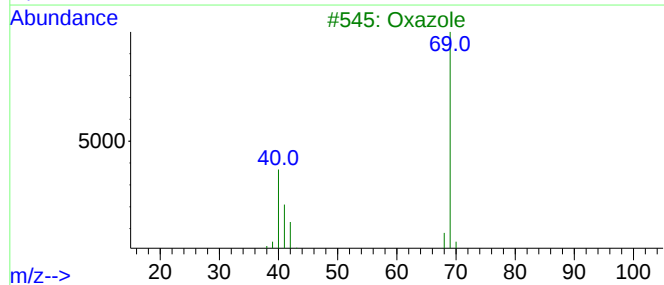
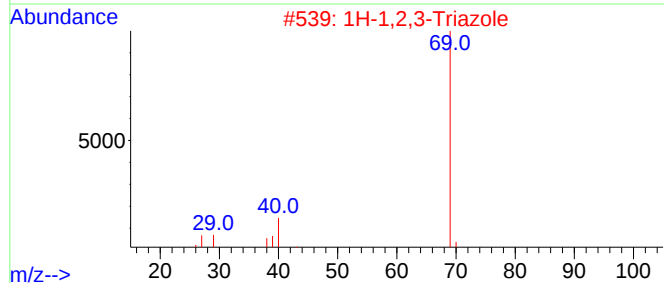
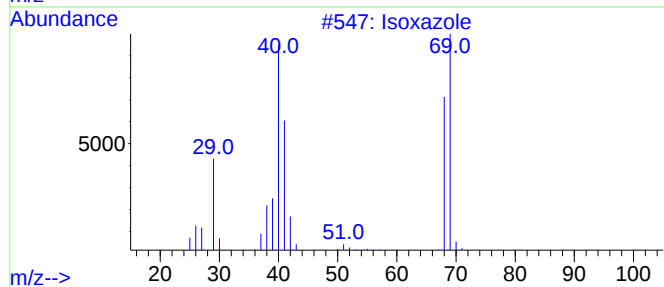
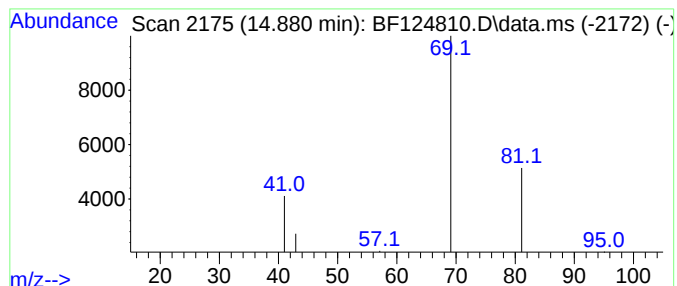
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.880 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	2.42 ng	5522	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoxazole	69	C3H3NO	000288-14-2	4
2			1H-1,2,3-Triazole	69	C2H3N3	000288-36-8	2
3			Oxazole	69	C3H3NO	000288-42-6	2
4			1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	2
5			2-Propynenitrile, 3-fluoro-	69	C3FN	032038-83-8	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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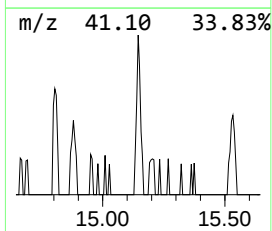
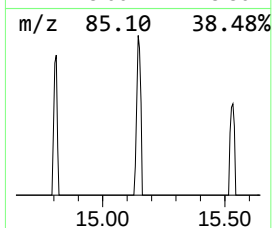
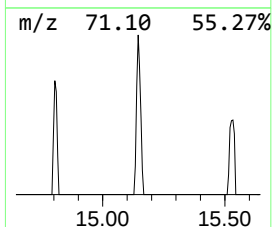
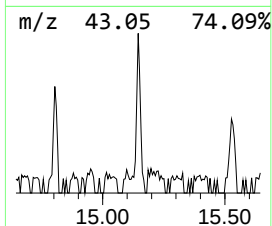
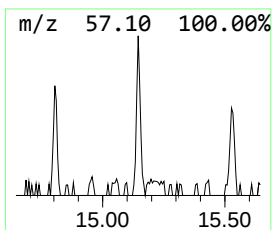
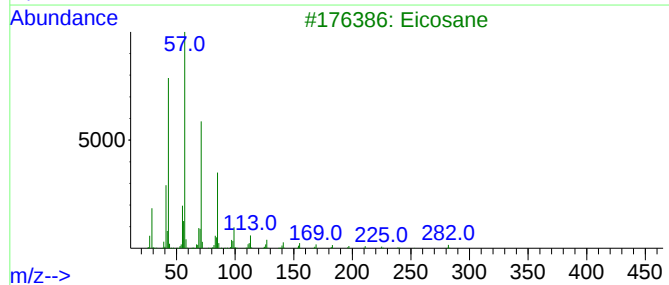
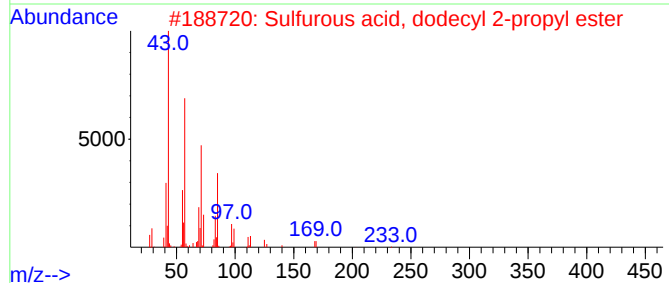
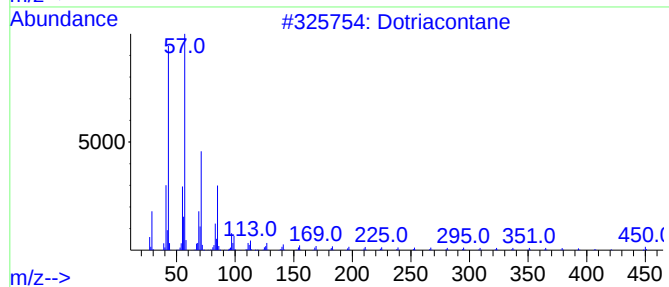
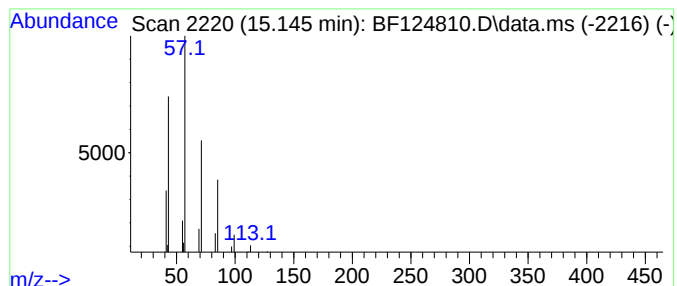
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Dotriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	9.90 ng	22597	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontane	451	C32H66	000544-85-4	78
2			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	78
3			Eicosane	282	C20H42	000112-95-8	72
4			Nonadecane	268	C19H40	000629-92-5	64
5			Heptadecane	240	C17H36	000629-78-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-078

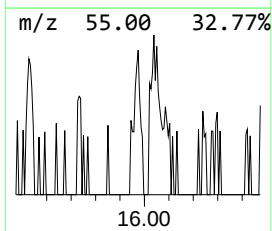
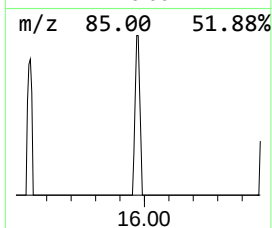
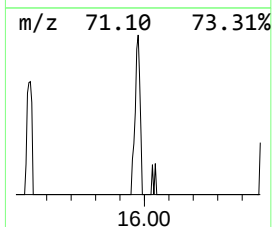
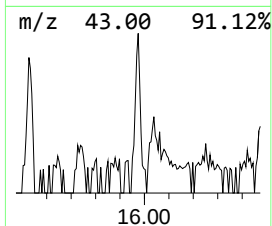
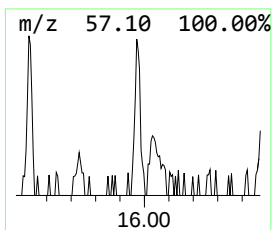
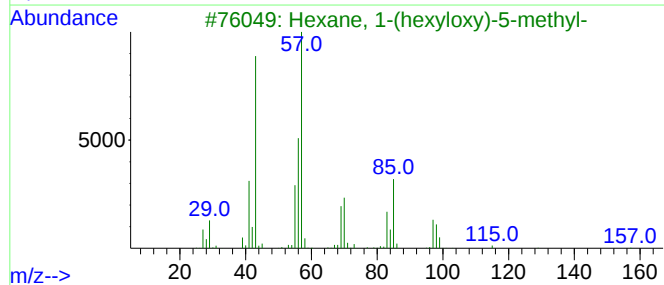
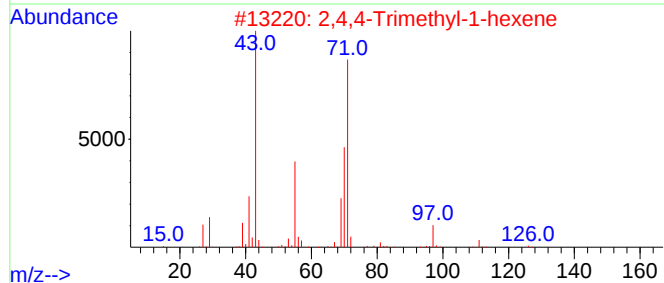
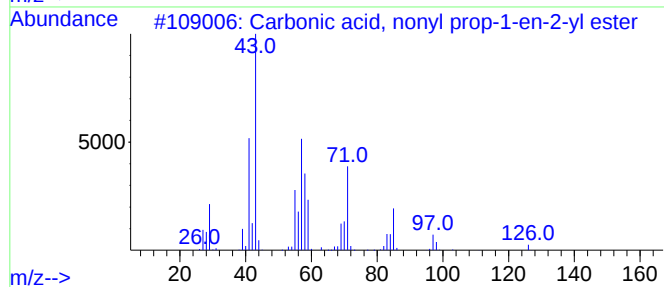
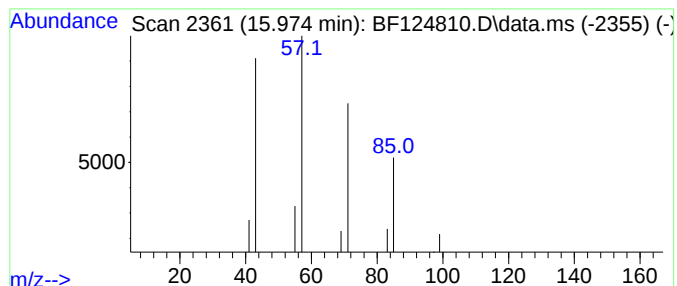
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown15.974 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	6.93 ng	15822	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	40
2			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	17
3			Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	16
4			Ether, heptyl hexyl	200	C13H28O	007289-40-9	12
5			Octadecane, 2,2,4,15,17,17-hexam...	591	C42H86	055470-97-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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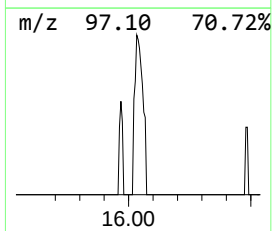
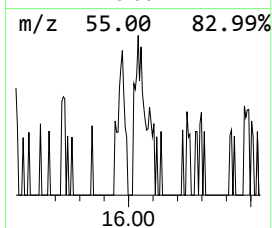
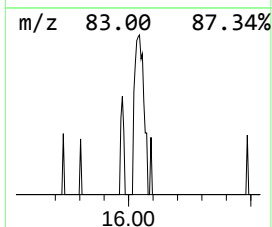
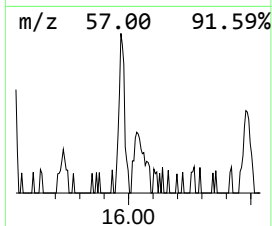
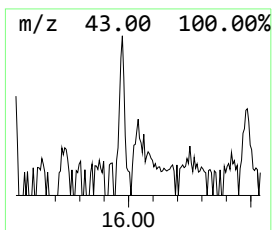
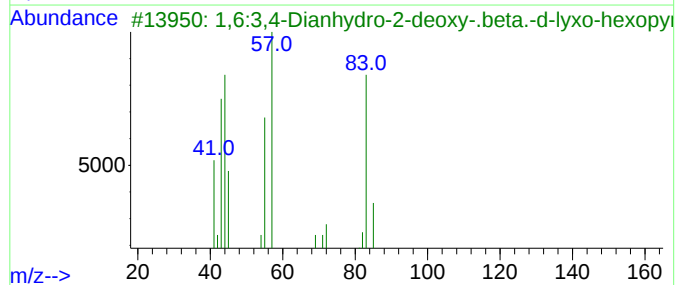
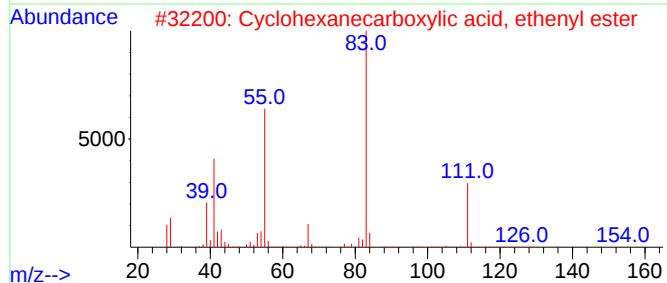
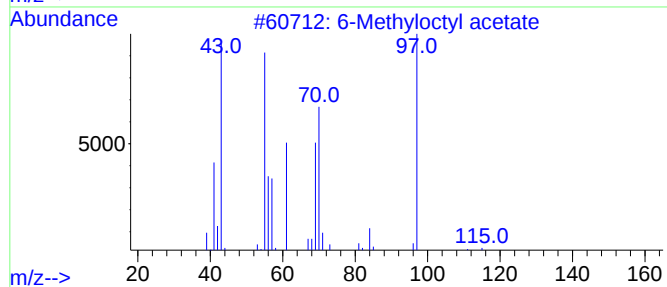
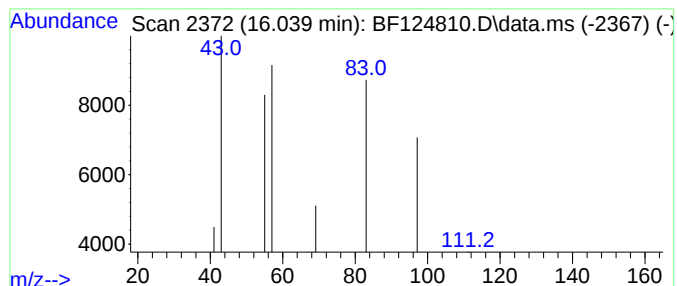
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown16.039 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	7.25 ng	16536	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	9
2			Cyclohexanecarboxylic acid, ethe...	154	C9H14O2	004840-76-0	9
3			1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	9
4			2-Acetyl-1-pyrroline	111	C6H9NO	085213-22-5	5
5			5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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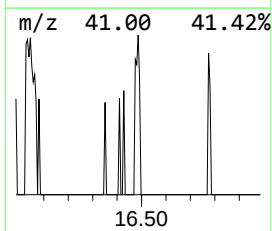
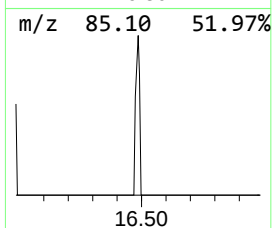
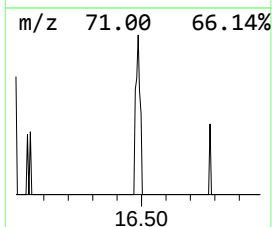
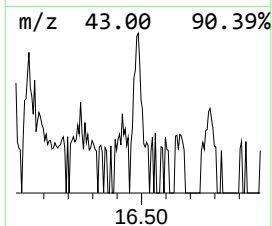
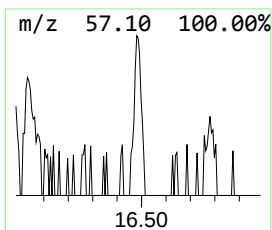
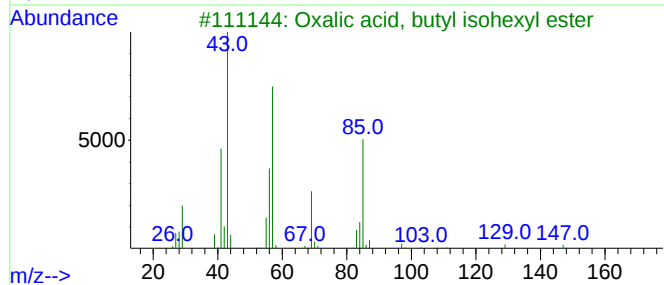
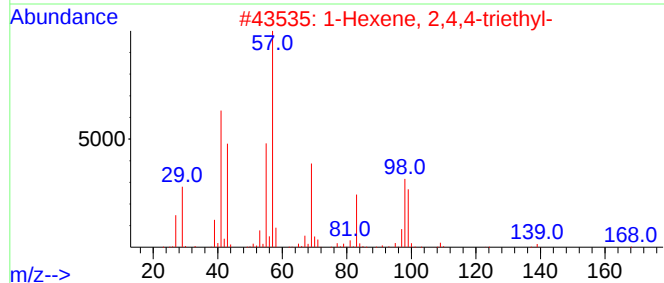
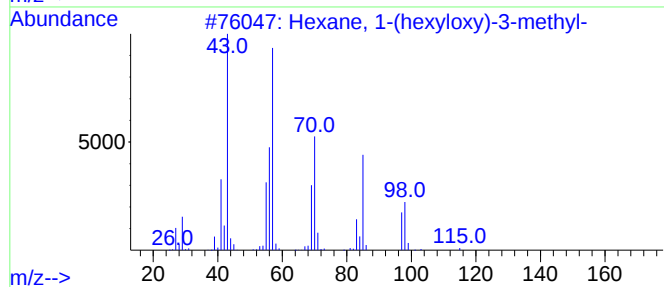
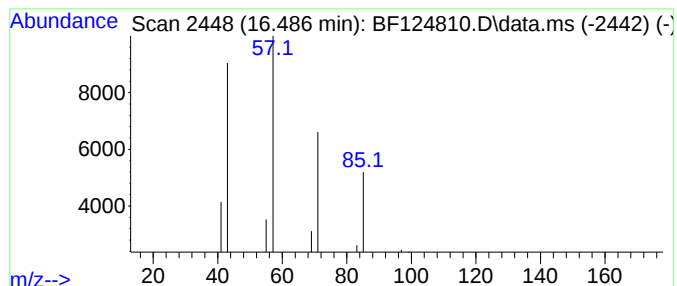
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown16.486 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.486	4.15 ng	9479	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 1-(hexyloxy)-3-methyl-	200	C13H28O	074421-18-4	25
2			1-Hexene, 2,4,4-triethyl-	168	C12H24	1000156-96-5	12
3			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	12
4			Cyclohexanecarboxylic acid, 1-(2...	284	C15H24O5	1000460-66-2	10
5			Octane, 2,5,6-trimethyl-	156	C11H24	062016-14-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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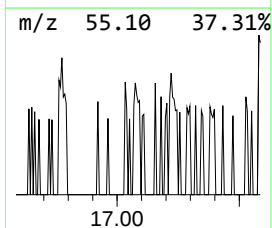
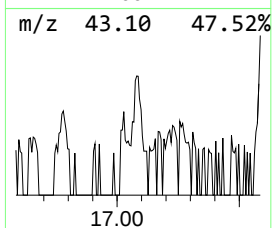
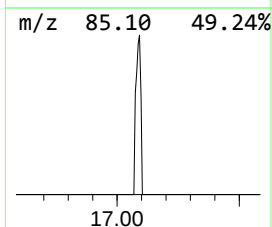
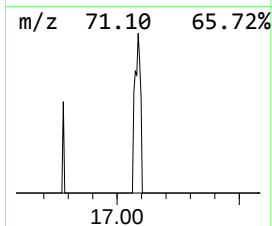
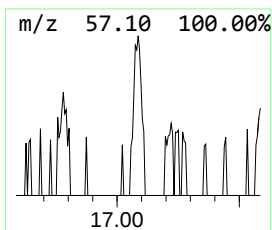
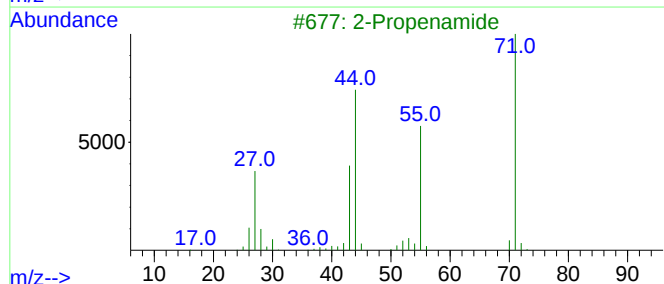
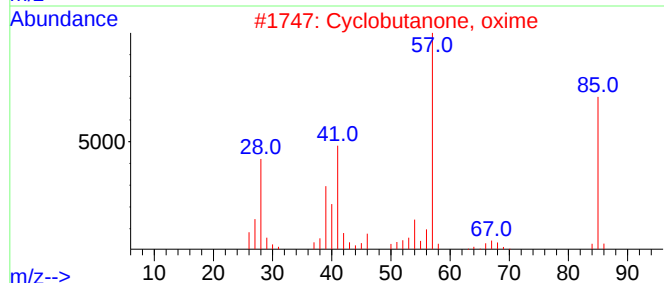
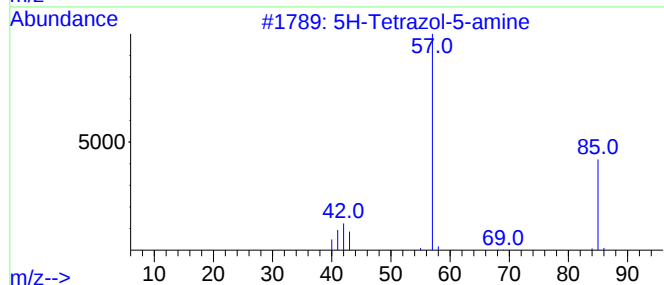
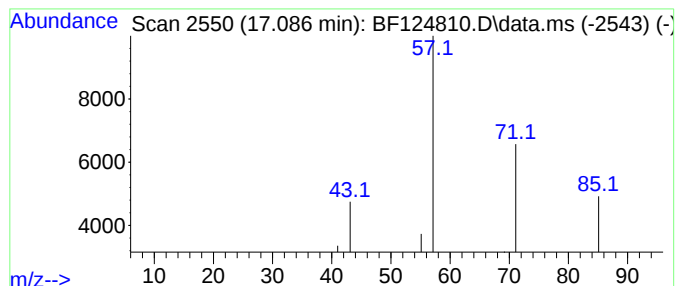
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown17.086 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.086	3.53 ng	8058	Perylene-d12	15.509

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
2		Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
3		2-Propenamide	71	C3H5NO	000079-06-1	4
4		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	4
5		Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-078

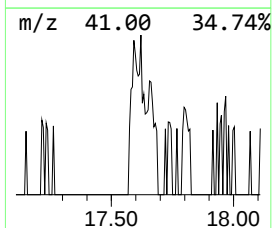
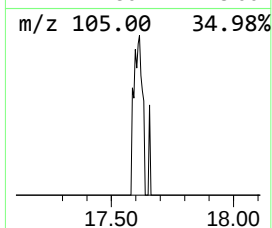
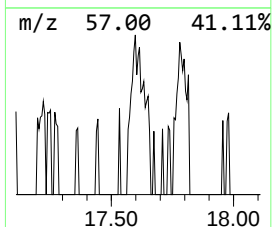
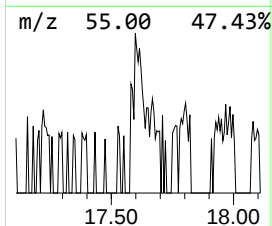
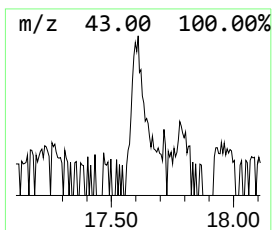
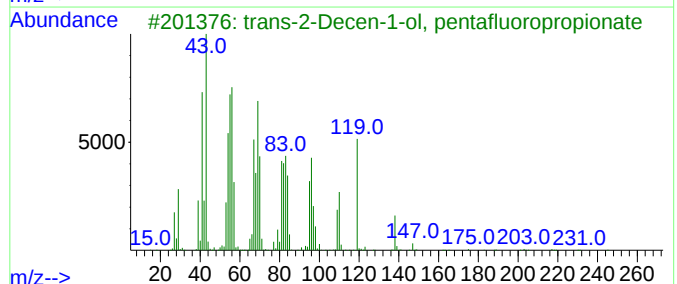
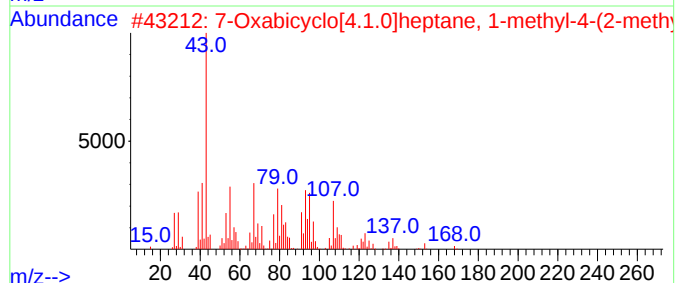
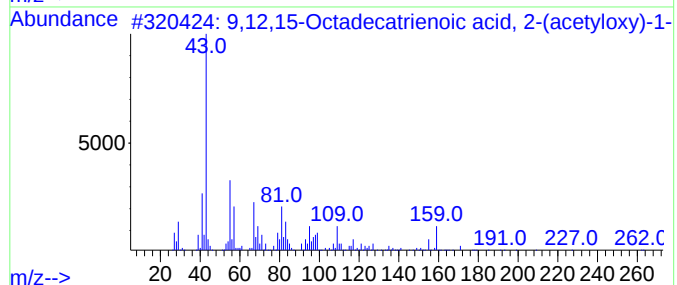
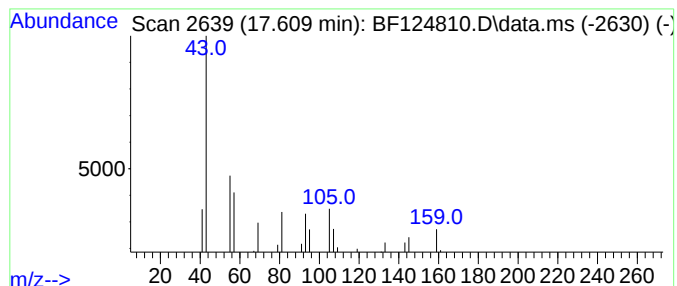
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown17.609 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.609	12.50 ng	28531	Perylene-d12	15.509

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, 2...	436	C25H40O6	055320-01-9	9	
2	7-Oxabicyclo[4.1.0]heptane, 1-me...	168	C10H16O2	000096-08-2	9	
3	trans-2-Decen-1-ol, pentafluorop...	302	C13H19F5O2	1000352-66-7	9	
4	Sobrero 8-acetate	212	C12H20O3	093133-02-9	7	
5	1H-Benzotriazole, 1-acetyl-	161	C8H7N3O	018773-93-8	4	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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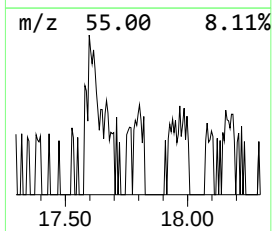
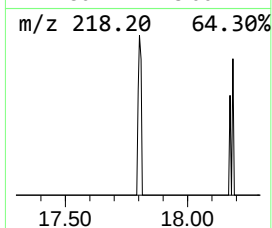
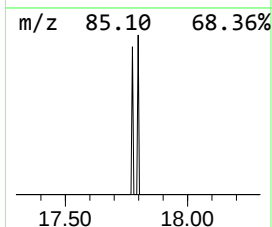
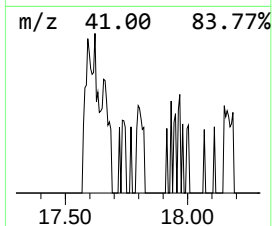
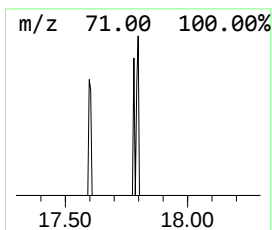
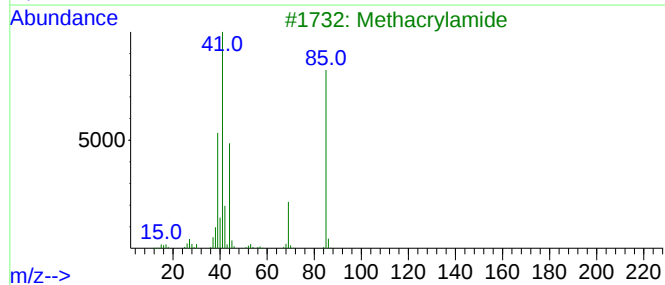
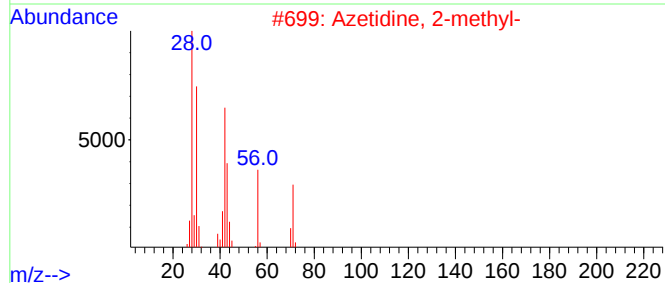
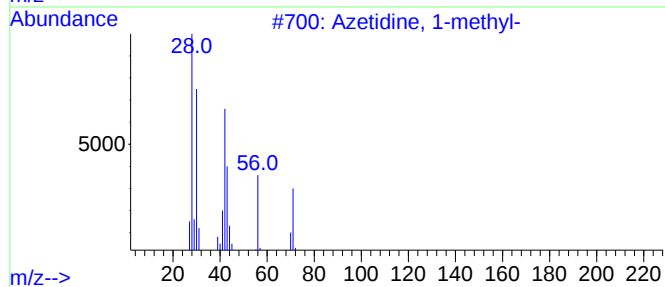
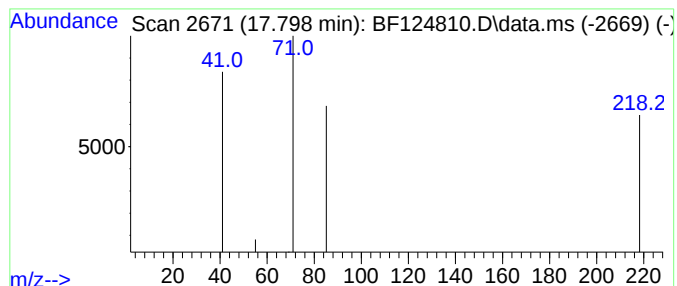
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown17.798 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.798	2.41 ng	5506	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	4
2			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	4
3			Methacrylamide	85	C4H7NO	000079-39-0	4
4			trans-Crotonamide	85	C4H7NO	000625-37-6	4
5			2-Pyrrolidinone	85	C4H7NO	000616-45-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-078

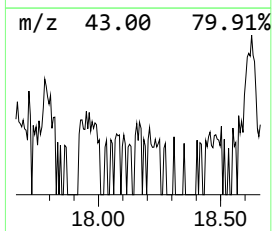
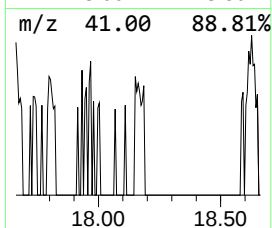
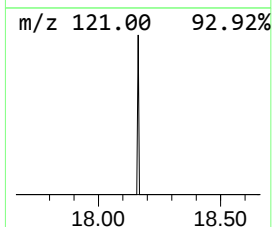
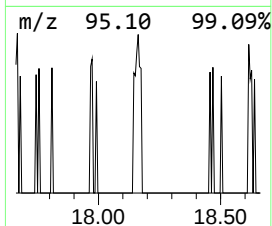
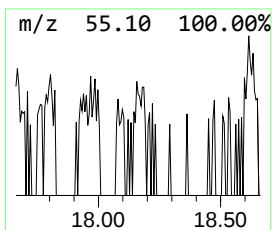
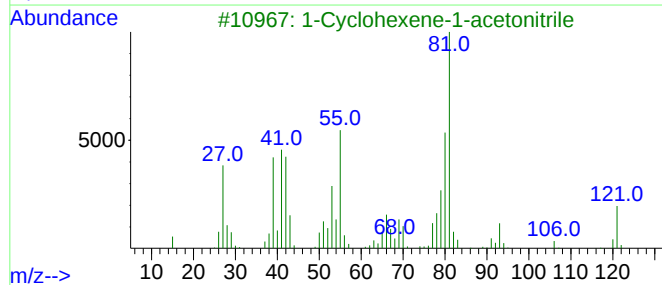
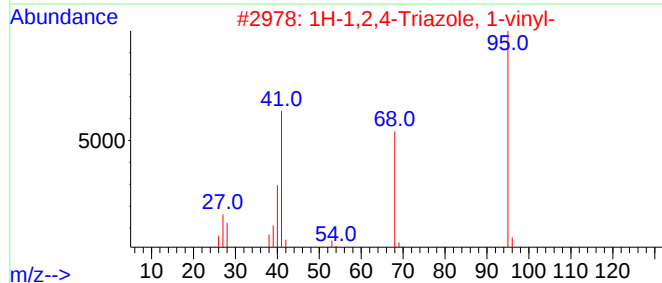
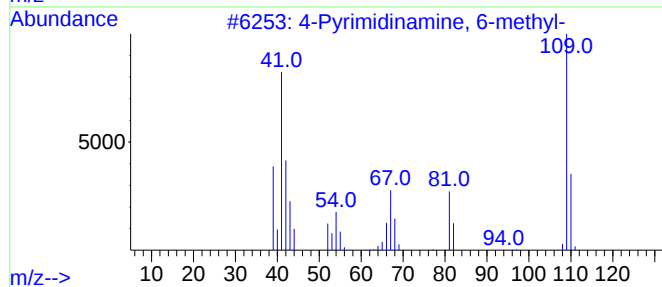
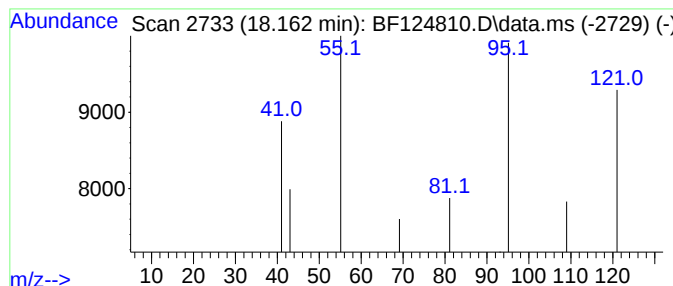
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown18.162 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.162	2.73 ng	6232	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyrimidinamine, 6-methyl-			109	C5H7N3	003435-28-7	4
2	1H-1,2,4-Triazole, 1-vinyl-			95	C4H5N3	002764-83-2	4
3	1-Cyclohexene-1-acetonitrile			121	C8H11N	006975-71-9	3
4	5-Hexenenitrile, 2-methyl-			109	C7H11N	030316-00-8	3
5	Phenol, o-amino-			109	C6H7NO	000095-55-6	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124810.D
Acq On : 28 Jul 2021 00:19
Operator : JU/CG
Sample : M3171-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-078

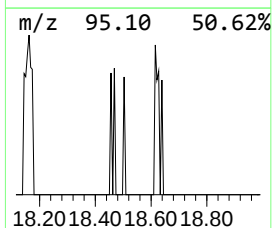
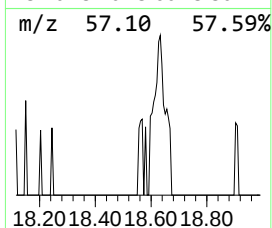
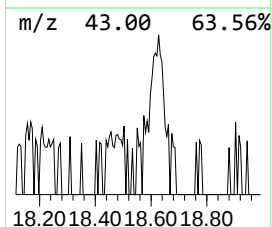
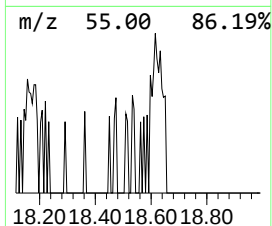
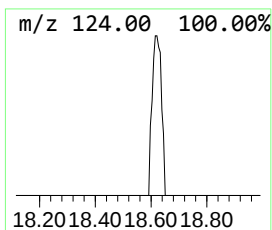
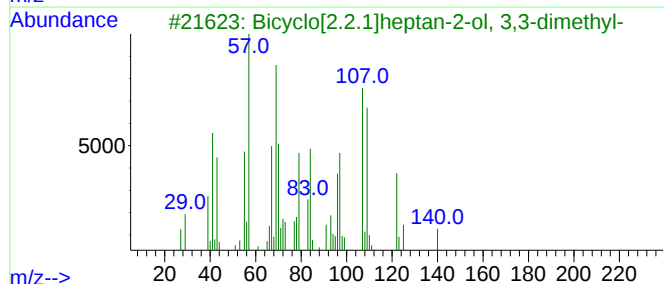
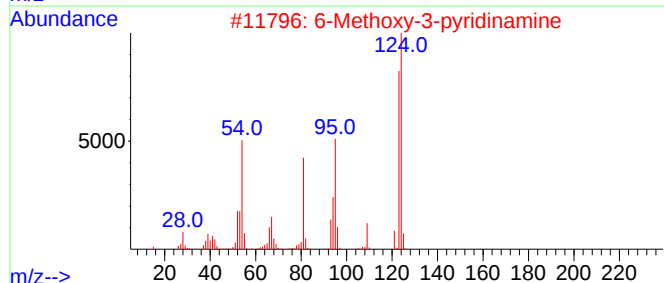
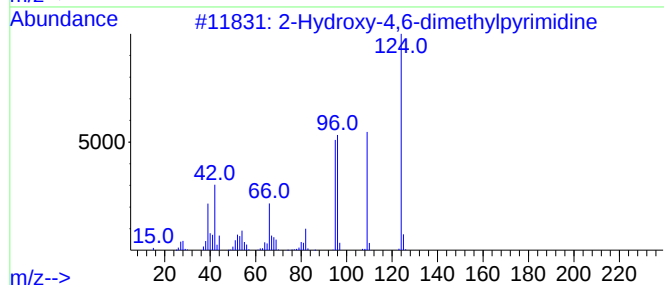
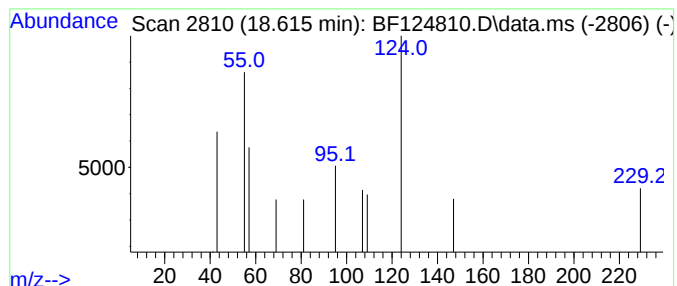
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown18.615 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.615	5.51 ng	12574	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-4,6-dimethylpyrimidine	124	C6H8N2O	1000476-61-0	32		
2	6-Methoxy-3-pyridinamine	124	C6H8N2O	006628-77-9	9		
3	Bicyclo[2.2.1]heptan-2-ol, 3,3-d...	140	C9H16O	005957-68-6	9		
4	3-Chloropropionic acid, 2,6-dime...	256	C14H21ClO2	1000299-21-8	9		
5	2H-Inden-2-one, octahydro-3a-met...	152	C10H16O	020379-99-1	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
 Data File : BF124810.D
 Acq On : 28 Jul 2021 00:19
 Operator : JU/CG
 Sample : M3171-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-078

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	5.4	ng	8991	1	6.869	33263	20.0
Ethanol, 2-(2-b...	8.051	6.5	ng	14928	2	8.151	46061	20.0
Dodecanoic acid	11.916	3.8	ng	10432	4	11.392	55504	20.0
unknown13.204	13.204	3.3	ng	5184	5	14.033	31136	20.0
unknown13.545	13.545	5.5	ng	8515	5	14.033	31136	20.0
Hexatriacontane	13.880	16.8	ng	26087	5	14.033	31136	20.0
Hexadecane	14.192	9.2	ng	14325	5	14.033	31136	20.0
1-Iodo-2-methyl...	14.498	11.3	ng	17630	5	14.033	31136	20.0
unknown14.527	14.527	5.8	ng	9041	5	14.033	31136	20.0
Sulfurous acid,...	14.804	6.4	ng	14565	6	15.509	45637	20.0
unknown14.880	14.880	2.4	ng	5522	6	15.509	45637	20.0
Dotriacontane	15.145	9.9	ng	22597	6	15.509	45637	20.0
unknown15.974	15.974	6.9	ng	15822	6	15.509	45637	20.0
unknown16.039	16.039	7.3	ng	16536	6	15.509	45637	20.0
unknown16.486	16.486	4.2	ng	9479	6	15.509	45637	20.0
unknown17.086	17.086	3.5	ng	8058	6	15.509	45637	20.0
unknown17.609	17.609	12.5	ng	28531	6	15.509	45637	20.0
unknown17.798	17.798	2.4	ng	5506	6	15.509	45637	20.0
unknown18.162	18.162	2.7	ng	6232	6	15.509	45637	20.0
unknown18.615	18.615	5.5	ng	12574	6	15.509	45637	20.0