

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
 Data File : BF124102.D
 Acq On : 27 May 2021 20:32
 Operator : JU/CG
 Sample : M2539-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-073

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-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124102.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	4	11	18	rVB	545580	702645	70.80%	7.089%
2	2.258	25	29	34	rBV2	11876	16971	1.71%	0.171%
3	5.093	508	511	517	rVB2	24837	28827	2.90%	0.291%
4	5.498	575	580	583	rBV	967382	878352	88.51%	8.862%
5	6.504	746	751	754	rBV	980769	888244	89.50%	8.962%
6	6.875	811	814	818	rBB	338986	257691	25.97%	2.600%
7	7.440	905	910	913	rBV	705975	637289	64.22%	6.430%
8	8.057	1013	1015	1028	rBV	57140	77767	7.84%	0.785%
9	8.157	1028	1032	1036	rVB	362866	317637	32.01%	3.205%
10	9.234	1211	1215	1218	rBV	1330485	992406	100.00%	10.012%
11	9.916	1327	1331	1334	rBV	415977	338880	34.15%	3.419%
12	10.698	1461	1464	1468	rBV	698023	595024	59.96%	6.003%
13	10.816	1480	1484	1489	rBV	17502	20530	2.07%	0.207%
14	11.398	1580	1583	1586	rBV	336765	295306	29.76%	2.979%
15	11.922	1669	1672	1675	rBV2	20676	19290	1.94%	0.195%
16	12.657	1794	1797	1802	rVB2	33381	33773	3.40%	0.341%
17	12.986	1849	1853	1856	rBV	915625	736664	74.23%	7.432%
18	13.216	1887	1892	1898	rBV6	13381	26815	2.70%	0.271%
19	13.386	1919	1921	1925	rBV5	11187	15786	1.59%	0.159%
20	13.433	1925	1929	1931	rVV4	16269	26371	2.66%	0.266%
21	13.492	1936	1939	1941	rVB2	27042	27887	2.81%	0.281%
22	13.563	1946	1951	1952	rBV5	29740	37680	3.80%	0.380%
23	13.639	1952	1964	1968	rBV10	106727	357040	35.98%	3.602%
24	13.886	2002	2006	2008	rBV2	44147	50353	5.07%	0.508%
25	13.910	2008	2010	2018	rVB4	51983	90600	9.13%	0.914%
26	14.039	2027	2032	2040	rVB	299738	312959	31.54%	3.157%
27	14.204	2056	2060	2063	rBV2	34223	36185	3.65%	0.365%
28	14.327	2078	2081	2085	rVB6	13671	14786	1.49%	0.149%
29	14.510	2109	2112	2116	rVB	76410	67968	6.85%	0.686%
30	14.569	2116	2122	2131	rBV10	38323	98805	9.96%	0.997%
31	14.821	2162	2165	2168	rVB	45823	45560	4.59%	0.460%
32	14.898	2176	2178	2185	rVB4	23615	28755	2.90%	0.290%
33	14.968	2187	2190	2193	rVB5	19610	20148	2.03%	0.203%
34	15.168	2220	2224	2228	rBV	127090	133952	13.50%	1.351%
35	15.333	2250	2252	2258	rVB6	13867	19541	1.97%	0.197%
36	15.463	2269	2274	2279	rBV9	15540	38916	3.92%	0.393%

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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	15.527	2280	2285	2289	rVV3	242139	331686	33.42%	3.346%
38	15.557	2289	2290	2295	rVB	39744	32265	3.25%	0.326%
39	15.663	2306	2308	2316	rBV9	9809	13922	1.40%	0.140%
40	15.763	2321	2325	2329	rBV5	38789	50038	5.04%	0.505%
41	16.004	2361	2366	2373	rVB2	69819	109744	11.06%	1.107%
42	16.092	2376	2381	2383	rBV6	22179	39949	4.03%	0.403%
43	16.245	2405	2407	2410	rBV4	15287	16510	1.66%	0.167%
44	16.292	2410	2415	2421	rVB7	21725	50041	5.04%	0.505%
45	16.527	2449	2455	2459	rBV6	25731	44844	4.52%	0.452%
46	16.827	2500	2506	2510	rVB5	31045	57086	5.75%	0.576%
47	17.133	2554	2558	2564	rVB6	24961	46345	4.67%	0.468%
48	17.268	2579	2581	2584	rBV4	9855	13170	1.33%	0.133%
49	17.339	2586	2593	2599	rVV4	40002	105690	10.65%	1.066%
50	17.680	2643	2651	2652	rBV3	70927	127365	12.83%	1.285%
51	17.845	2677	2679	2687	rVB8	41669	87972	8.86%	0.888%
52	18.039	2704	2712	2717	rBV9	34857	87052	8.77%	0.878%
53	18.209	2734	2741	2750	rVB8	107688	293917	29.62%	2.965%
54	18.539	2793	2797	2801	rBV7	20149	25238	2.54%	0.255%
55	18.674	2815	2820	2822	rBV6	52943	91488	9.22%	0.923%

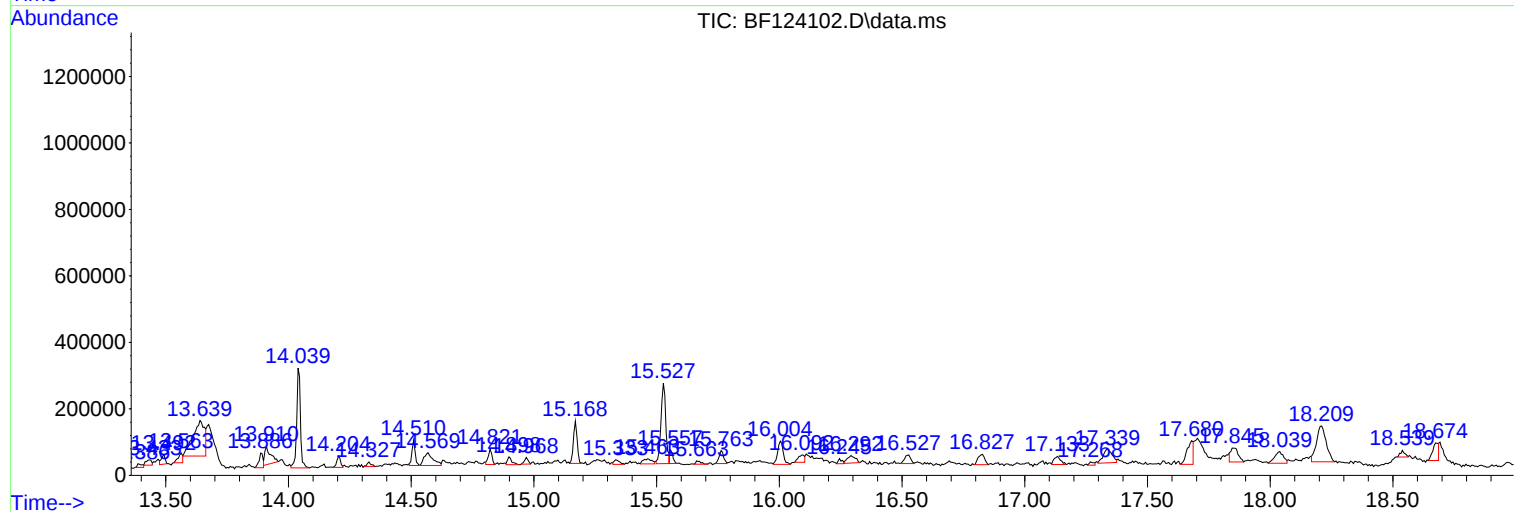
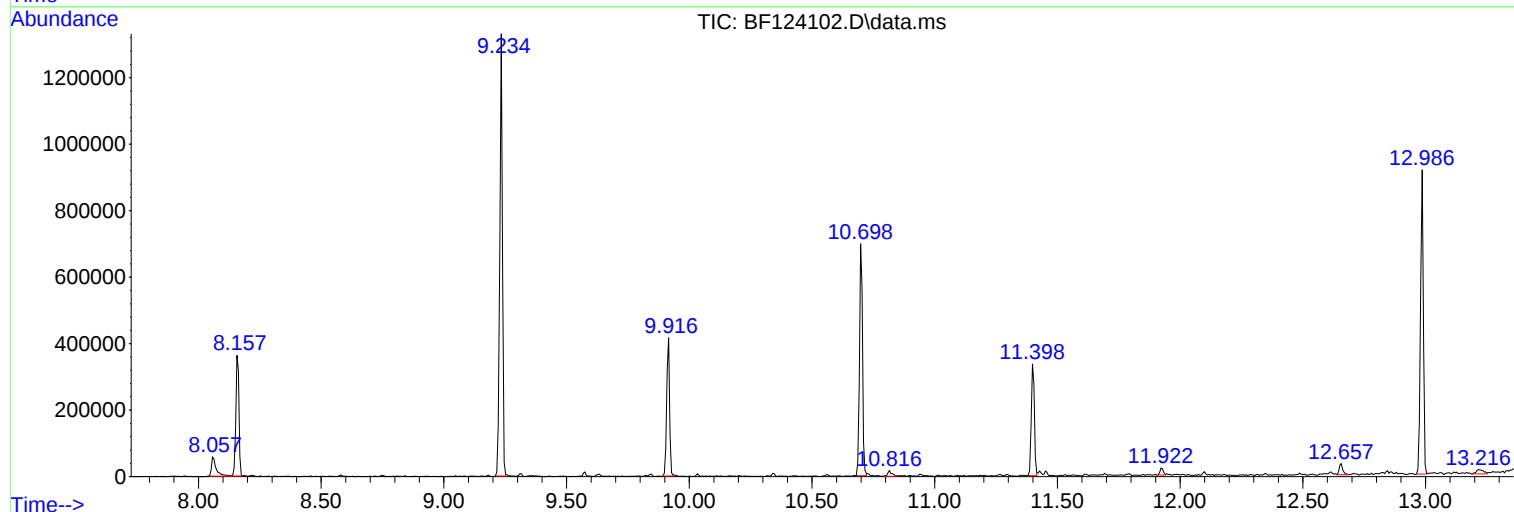
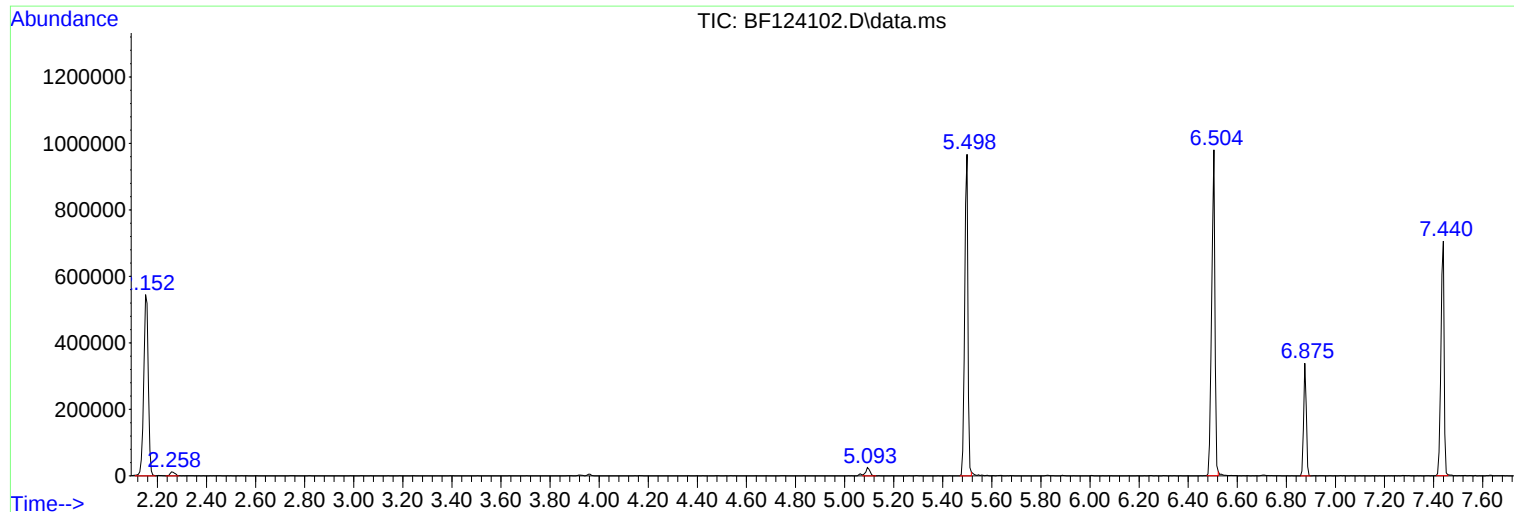
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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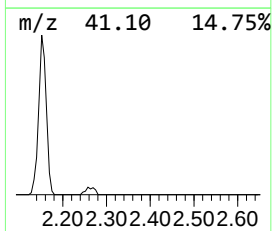
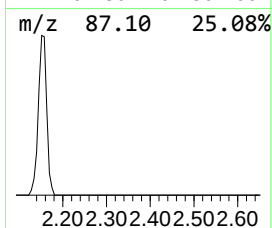
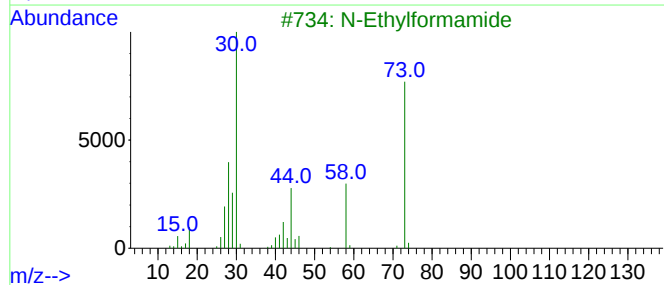
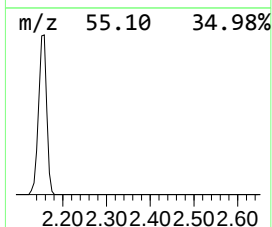
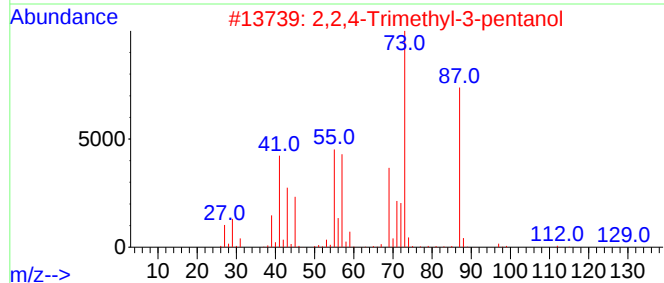
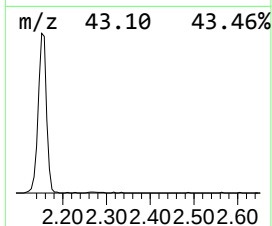
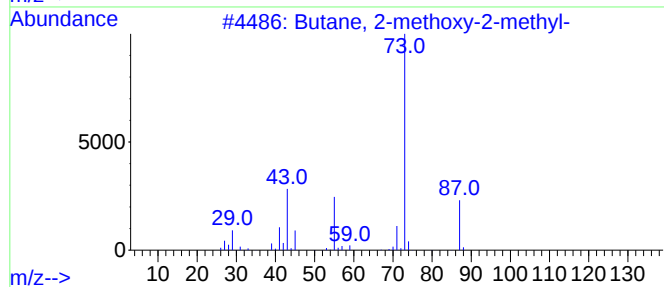
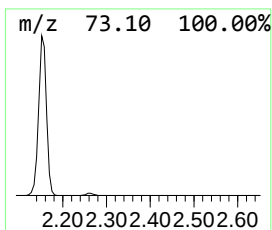
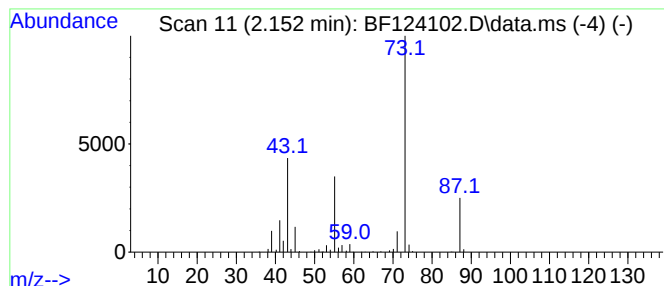
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.152	54.53 ng	702645	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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ClientSampleId :
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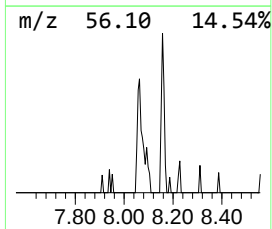
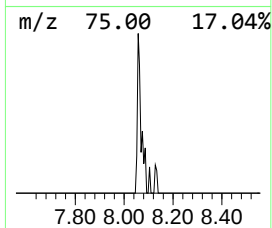
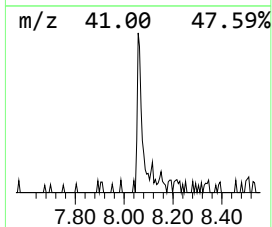
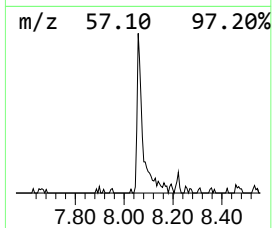
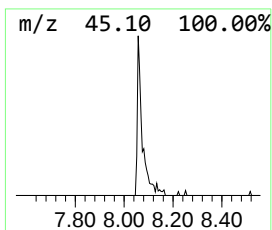
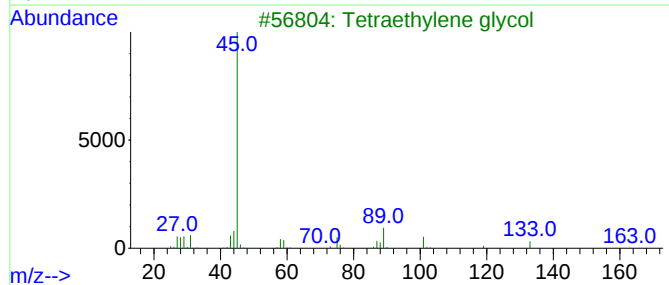
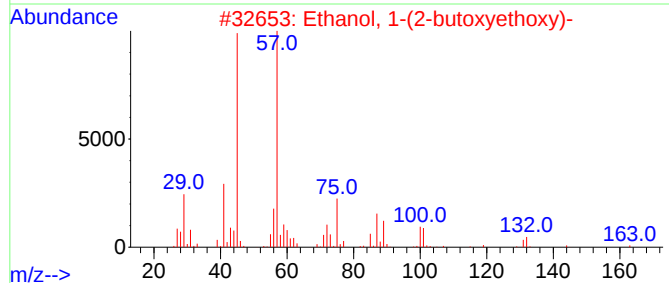
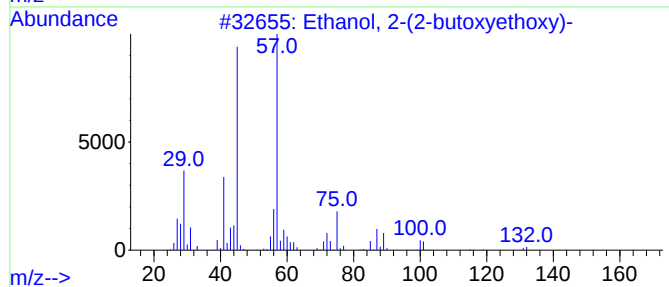
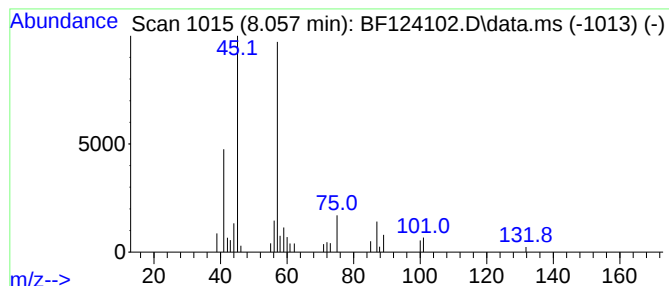
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.057	4.90 ng	77767	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Tetraethylene glycol	194	C8H18O5	000112-60-7	50
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50



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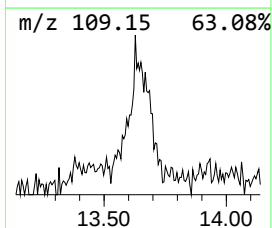
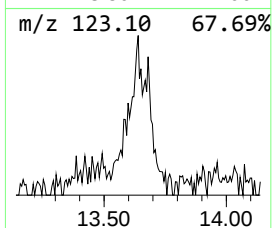
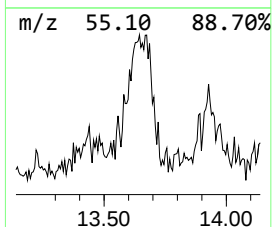
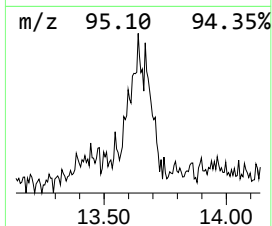
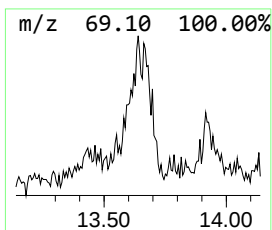
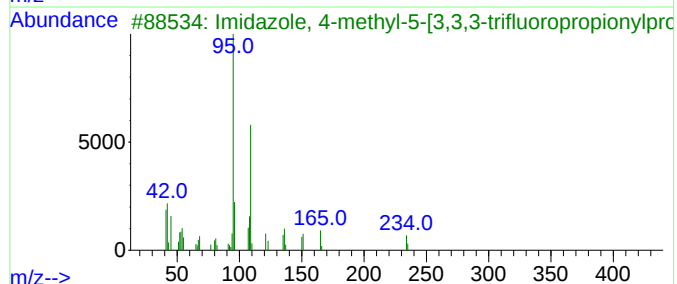
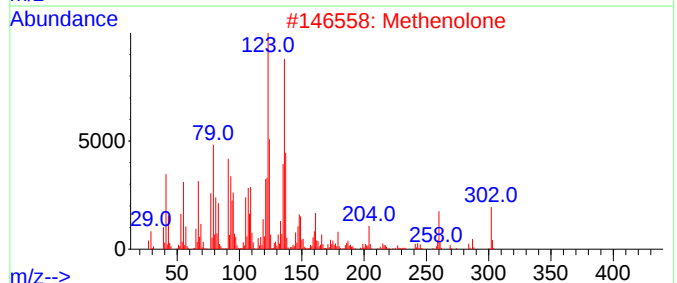
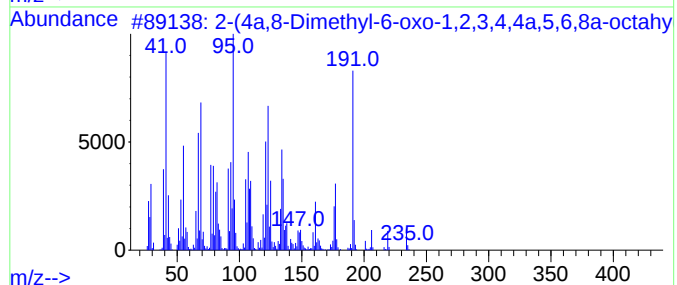
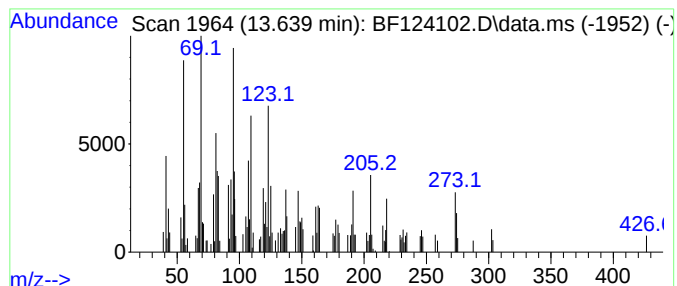
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown13.639 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.639	22.82 ng	357040	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	43		
2	Methenolone	302	C20H30O2	000153-00-4	41		
3	Imidazole, 4-methyl-5-[3,3,3-tri...	234	C10H13F3N2O	1000129-15-8	38		
4	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	30		
5	2,2-Dimethyl-3-[3,7,12-trimethyl...	426	C30H50O	1000195-23-3	30		



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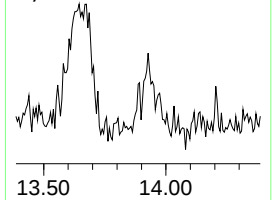
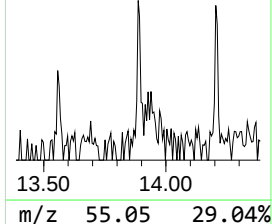
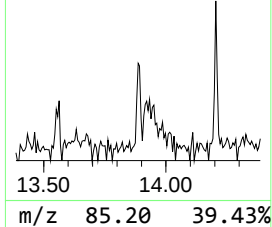
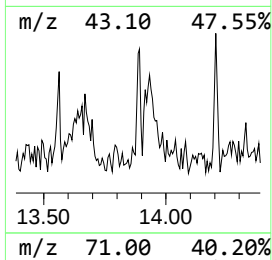
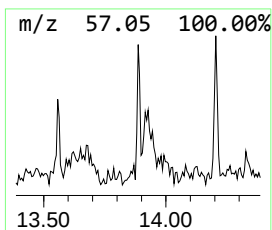
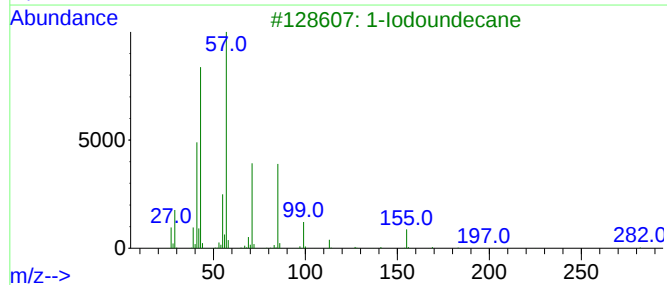
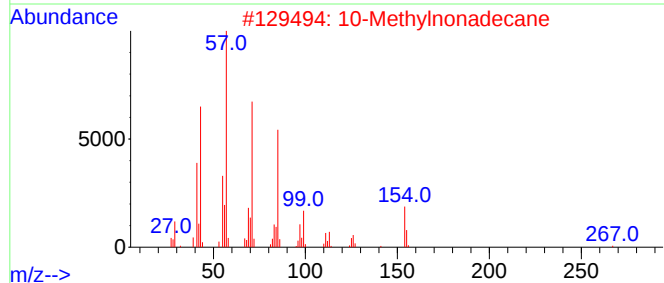
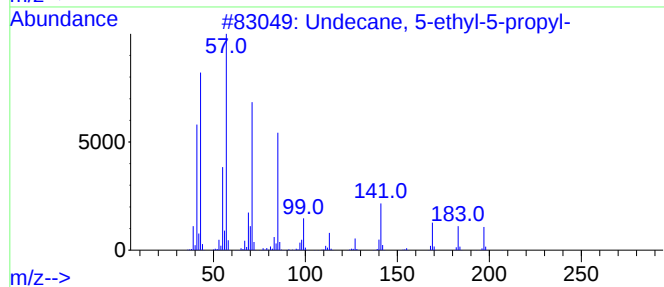
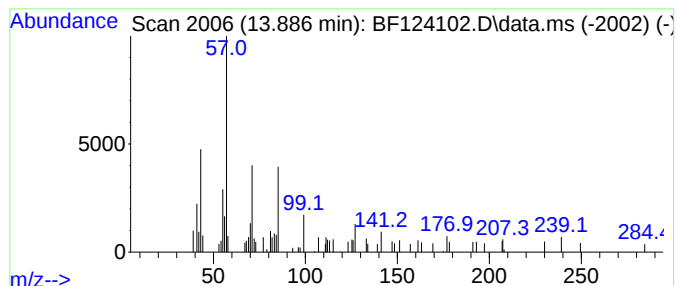
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Undecane, 5-ethyl-5-propyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.22 ng	50353	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 5-ethyl-5-propyl-	226	C16H34	002755-07-9	50
2			10-Methylnonadecane	282	C20H42	056862-62-5	50
3			1-Iodoundecane	282	C11H23I	004282-44-4	47
4			Pentadecane	212	C15H32	000629-62-9	47
5			Tridecane	184	C13H28	000629-50-5	47



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FK-PS-01-073

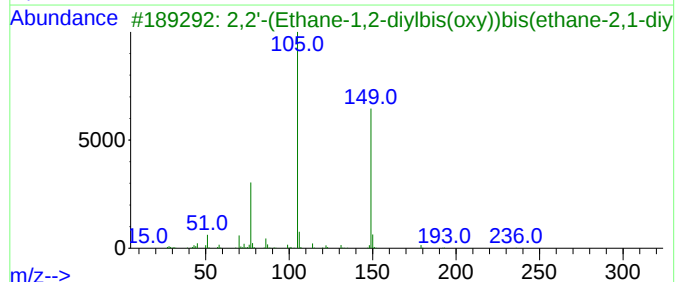
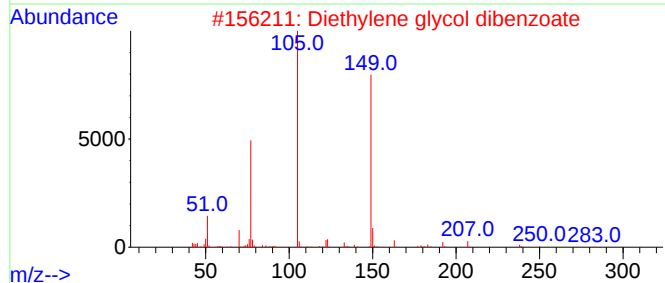
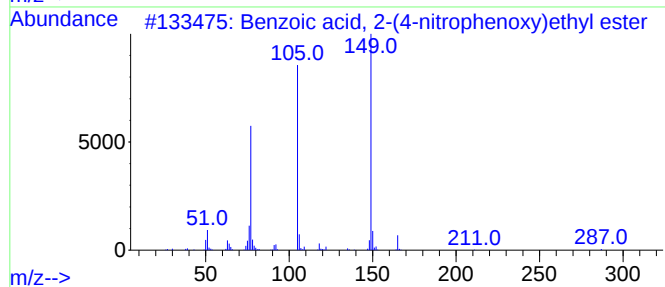
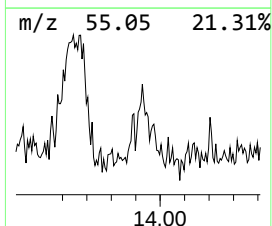
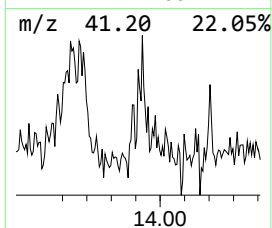
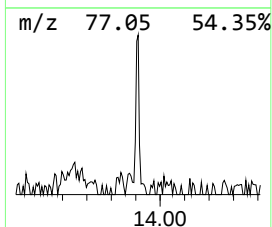
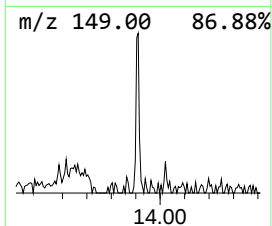
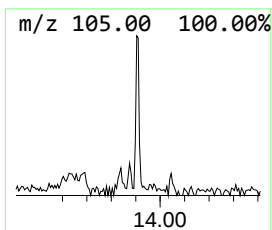
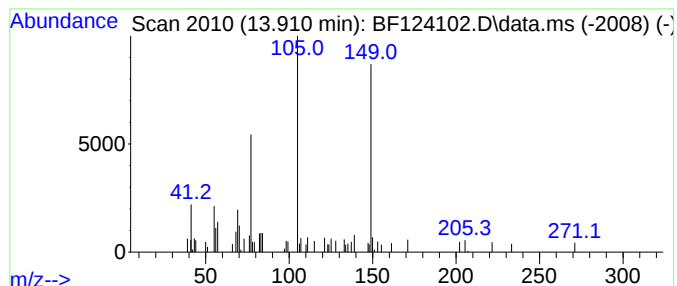
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzoic acid, 2-(4-nitrophe... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	5.79 ng	90600	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	50
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	50
3			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	50
4			Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	50
5			Phthalic acid, isobutyl 1-methox...	392	C23H36O5	1000315-39-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-073

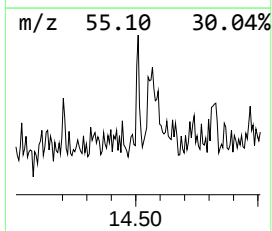
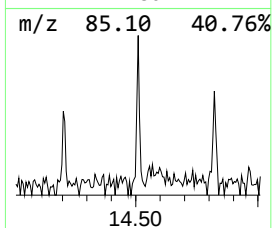
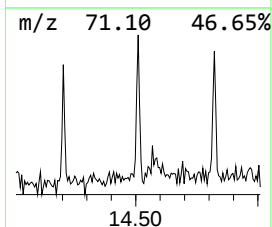
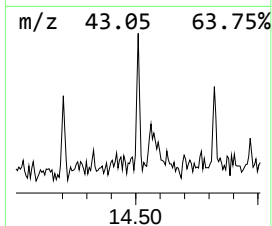
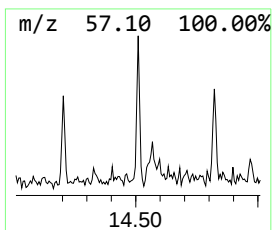
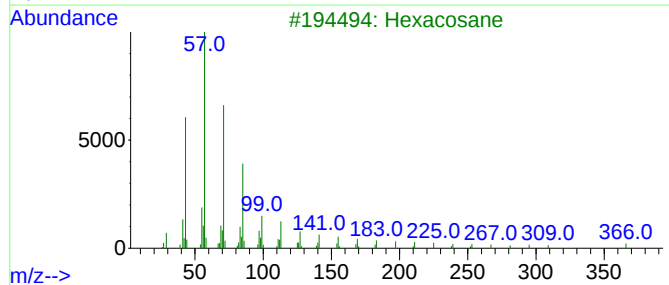
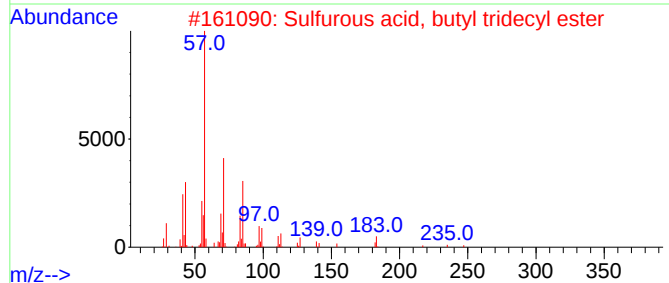
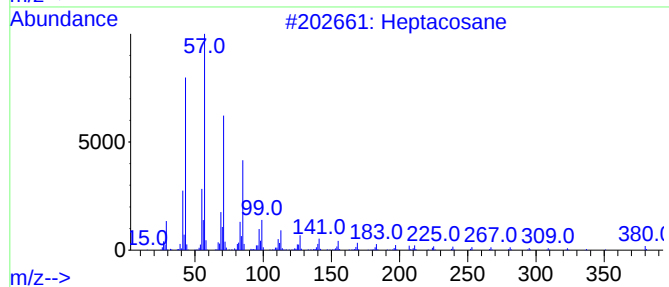
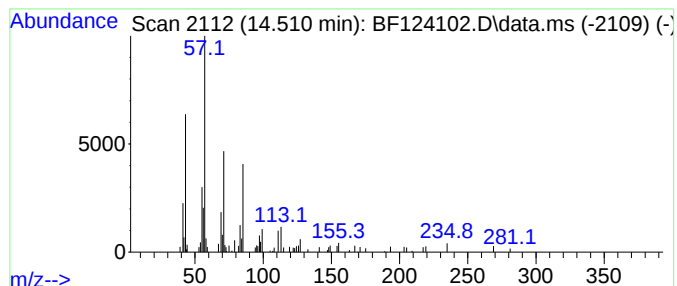
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.510	4.34 ng	67968	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	87
2			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	78
3			Hexacosane	366	C26H54	000630-01-3	72
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
5			Pentadecane	212	C15H32	000629-62-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-073

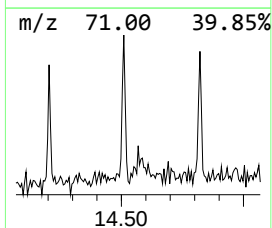
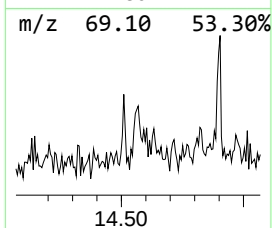
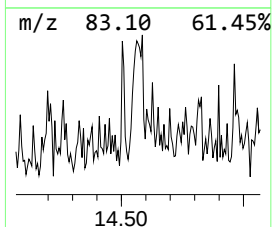
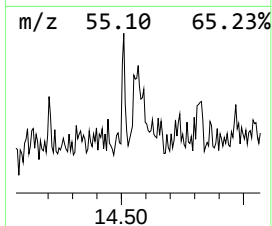
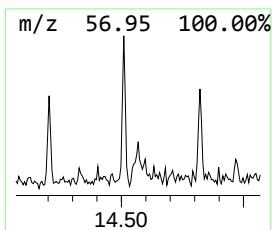
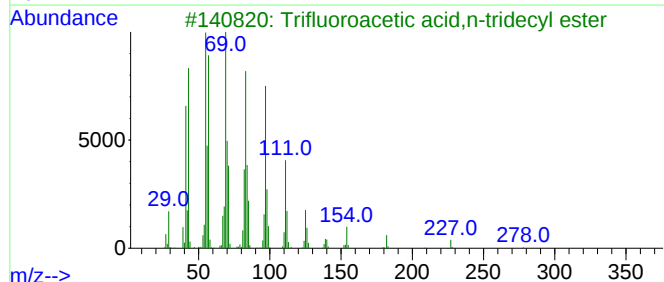
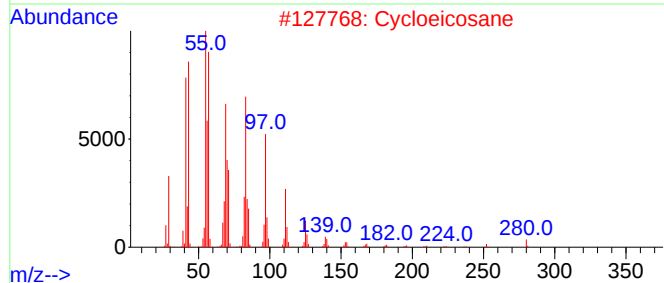
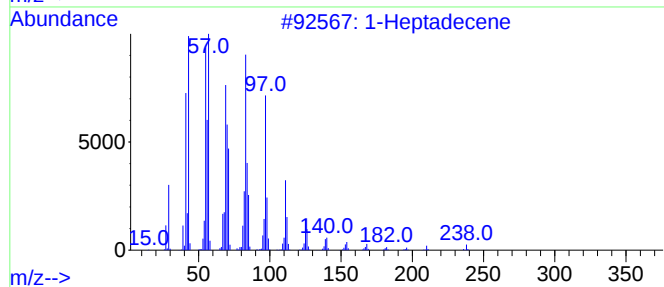
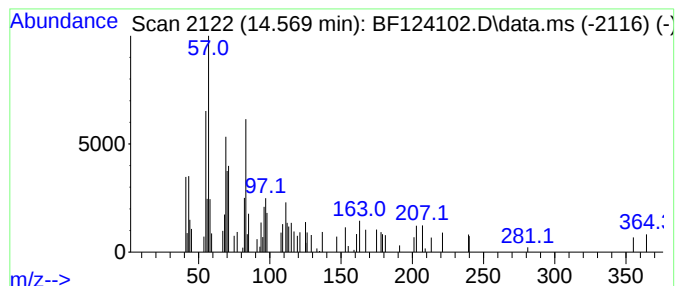
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown14.569 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.569	6.31 ng	98805	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptadecene	238	C17H34	006765-39-5	49
2			Cycloeicosane	280	C20H40	000296-56-0	47
3			Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	38
4			1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	35
5			1,22-Docosanediol	342	C22H46O2	022513-81-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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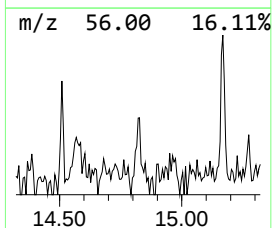
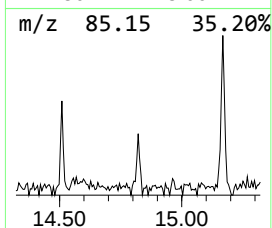
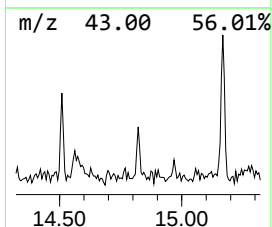
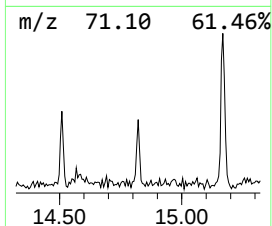
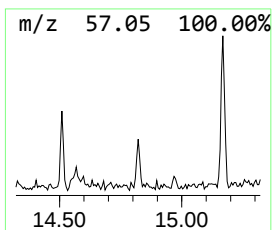
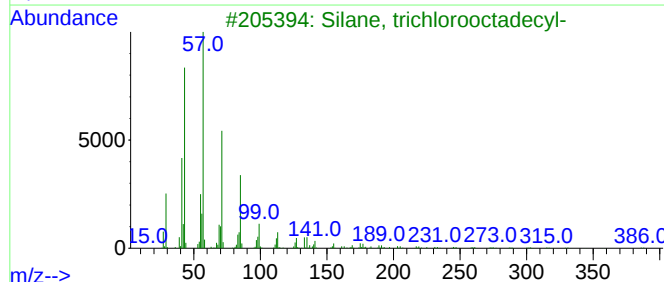
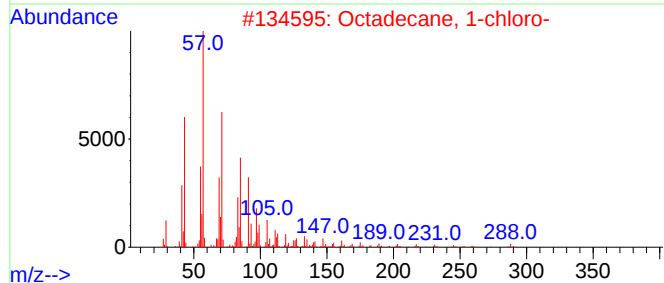
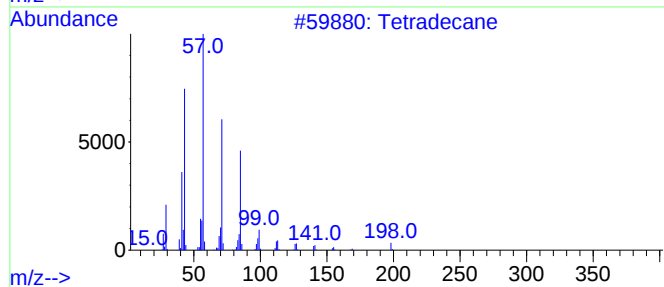
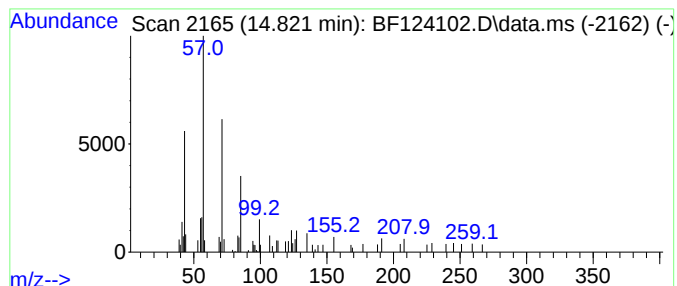
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Tetradecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	2.75 ng	45560	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	53
2			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	53
3			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	53
4			Hexadecane	226	C16H34	000544-76-3	53
5			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
Operator : JU/CG
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Misc :
ALS Vial : 15 Sample Multiplier: 1

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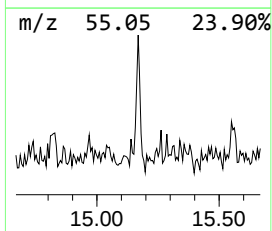
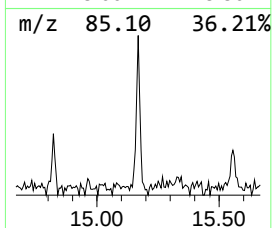
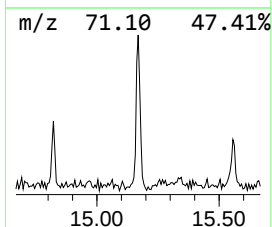
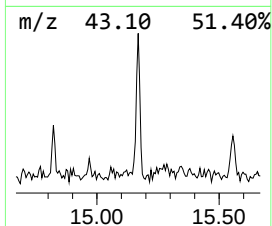
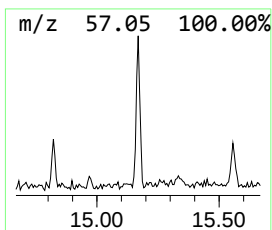
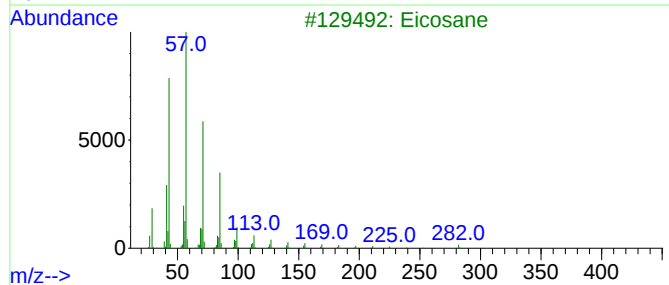
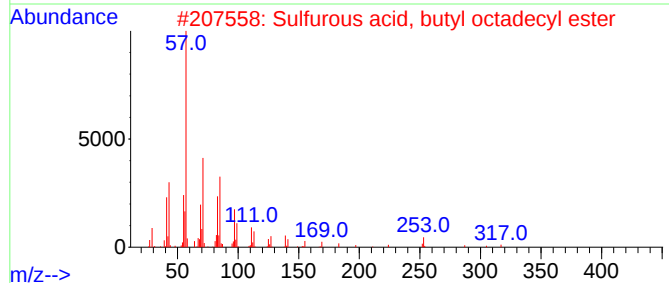
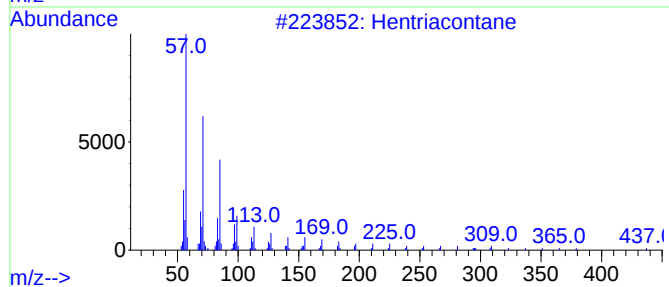
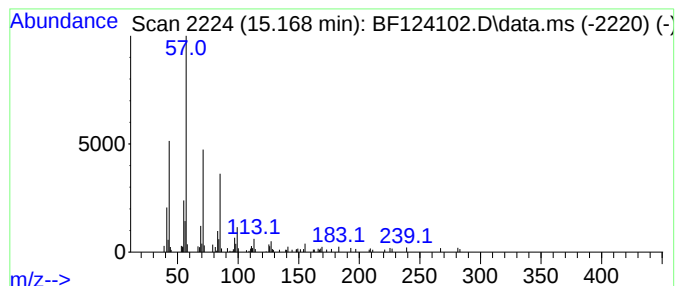
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.169	8.08 ng	133952	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	86
3			Eicosane	282	C20H42	000112-95-8	83
4			Eicosane, 3-methyl-	296	C21H44	006418-46-8	80
5			Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-073

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

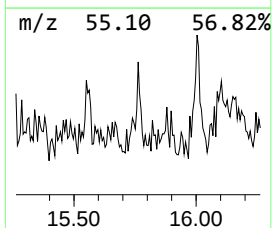
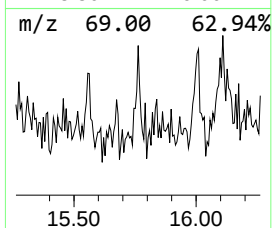
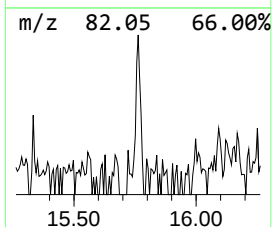
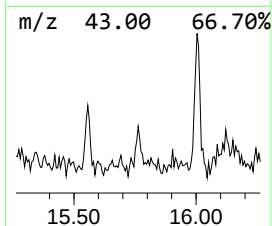
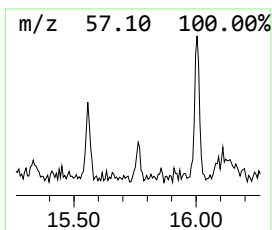
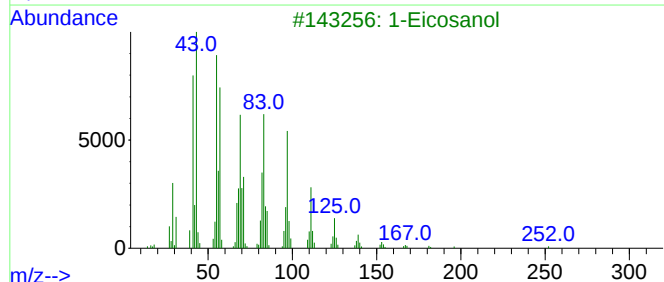
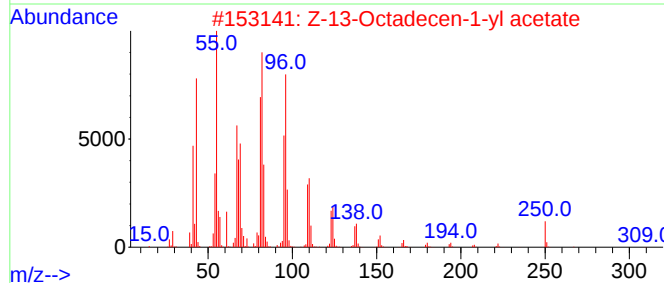
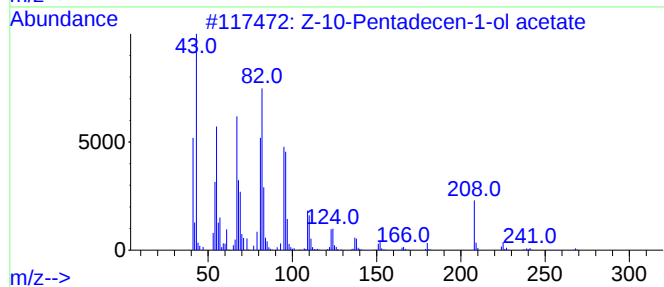
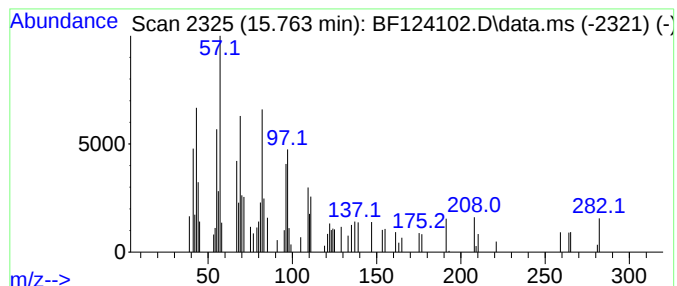
TIC Library : C:\DATABASE\NIST11.L

TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown15.762 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.762	3.02 ng	50038	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Z-10-Pentadecen-1-ol acetate	268	C17H32O2	1000130-85-0	49
2			Z-13-Octadecen-1-yl acetate	310	C20H38O2	060037-58-3	47
3			1-Eicosanol	298	C20H42O	000629-96-9	38
4			13-Methyl-12-tetradecen-1-ol ace...	268	C17H32O2	099798-78-4	38
5			Octadecanenitrile	265	C18H35N	000638-65-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
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ClientSampleId :
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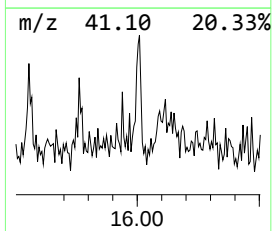
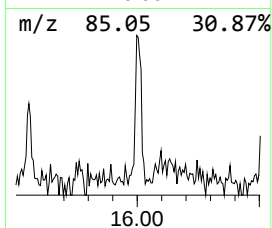
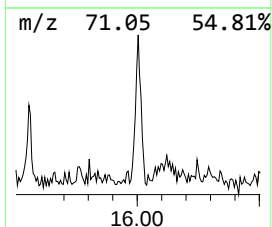
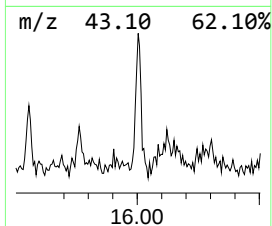
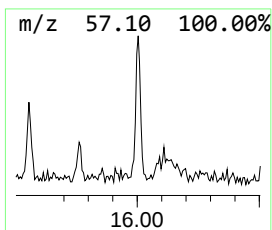
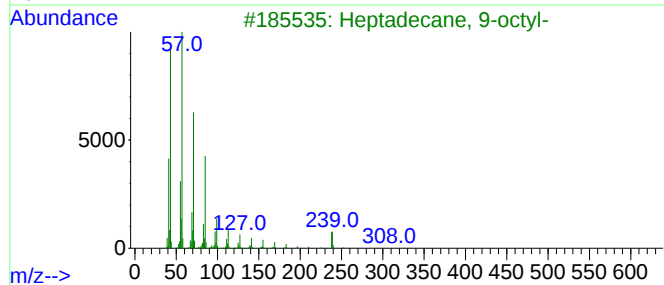
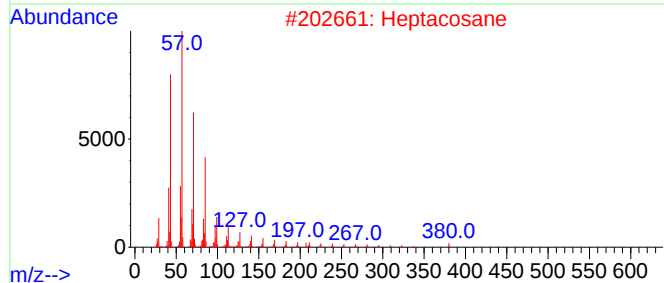
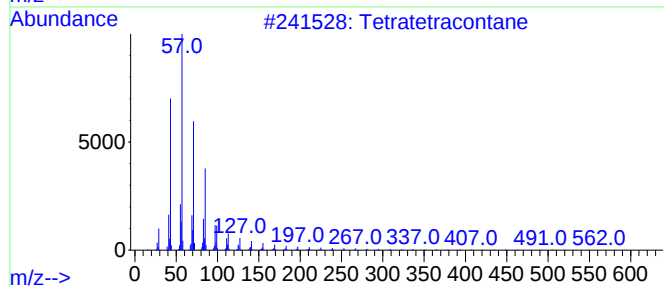
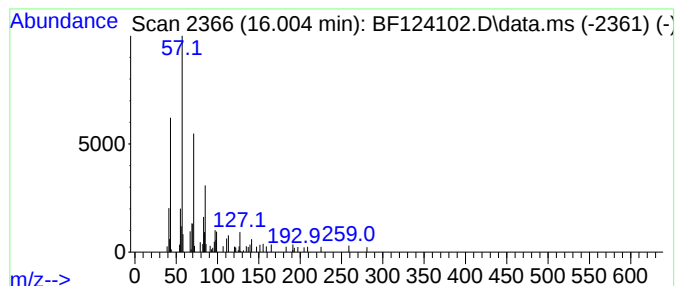
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	6.62 ng	109744	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Heptacosane	380	C27H56	000593-49-7	90
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
4			Hexatriacontane	507	C36H74	000630-06-8	83
5			Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	80



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Operator : JU/CG
Sample : M2539-01
Misc :
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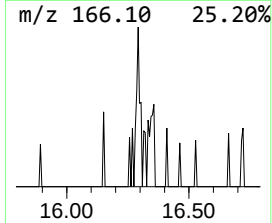
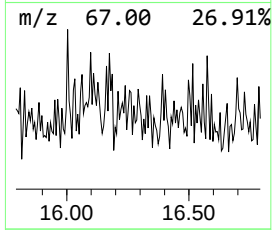
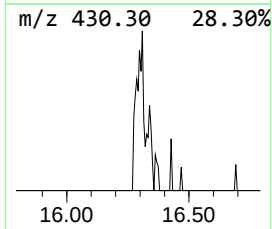
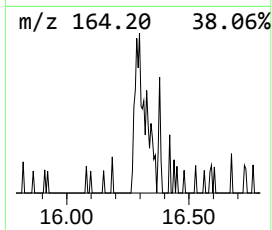
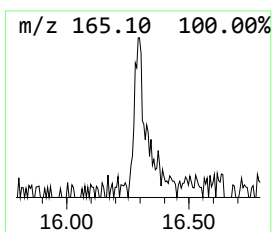
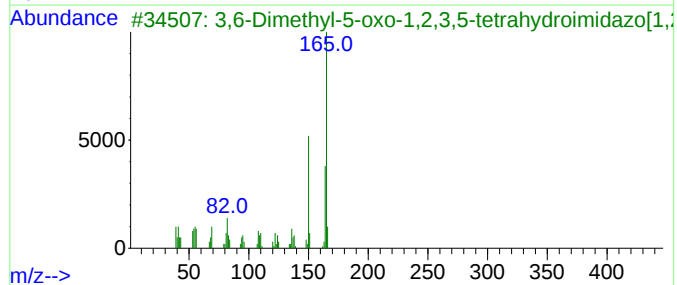
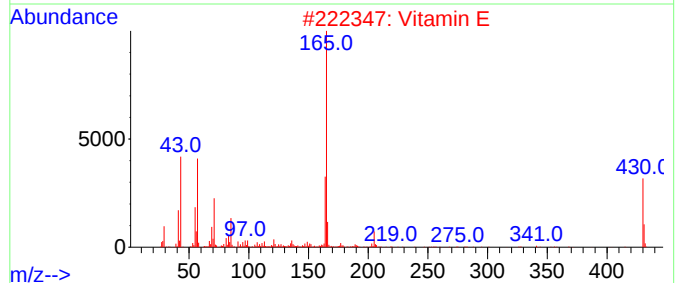
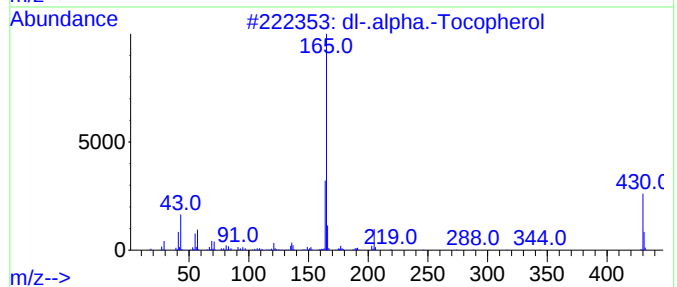
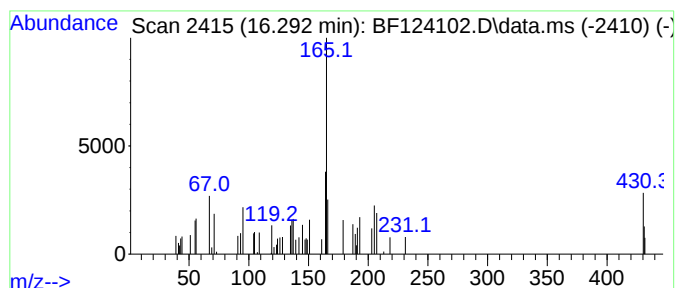
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 dl-.alpha.-Tocopherol Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.292	3.02 ng	50041	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-.alpha.-Tocopherol	430	C29H50O2	010191-41-0	64
2	Vitamin E	430	C29H50O2	000059-02-9	58
3	3,6-Dimethyl-5-oxo-1,2,3,5-tetra...	165	C8H11N3O	058910-42-2	47
4	Furo[3,4-c]pyridine-3,4(1H,5H)-d...	165	C8H7NO3	007472-18-6	43
5	1H-Purin-2-amine, 6-methoxy-	165	C6H7N5O	020535-83-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
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Misc :
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Instrument :
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ClientSampleId :
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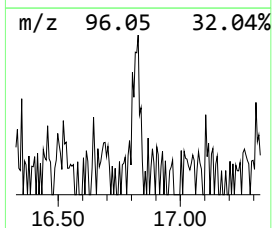
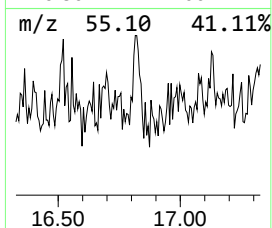
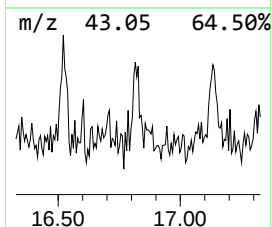
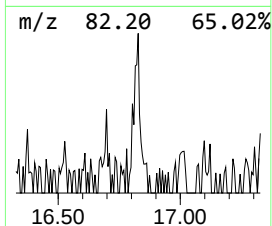
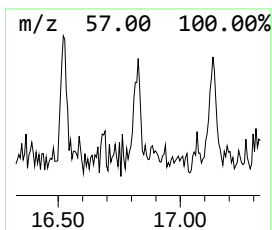
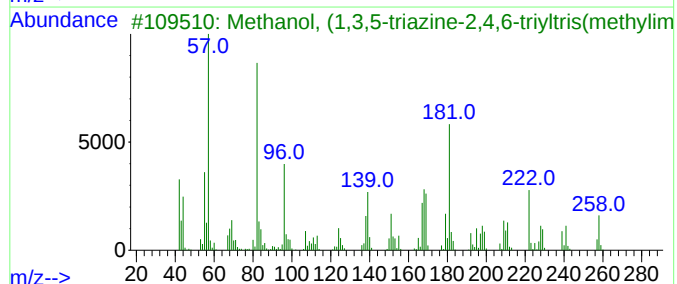
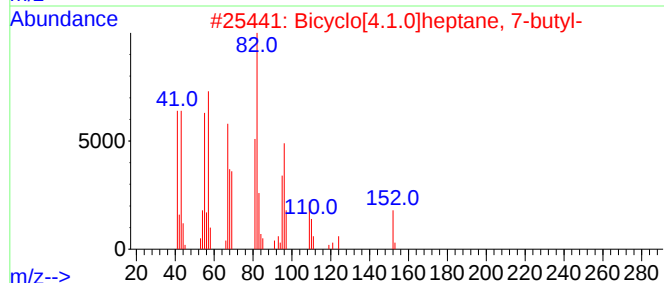
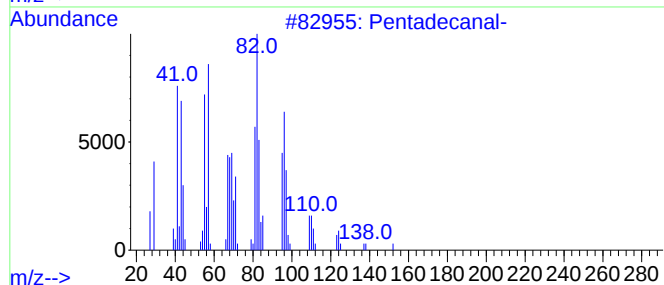
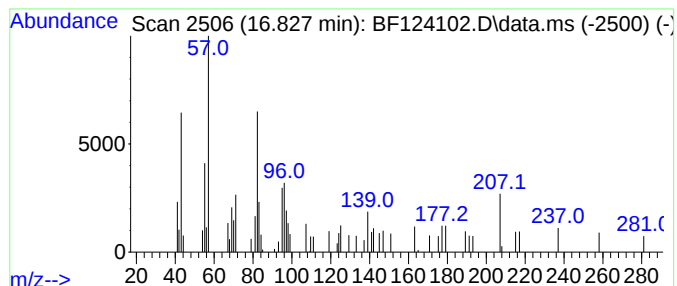
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown16.827 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.827	3.44 ng	57086	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanal-	226	C15H30O	002765-11-9	38
2			Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	37
3			Methanol, (1,3,5-triazine-2,4,6-...	258	C9H18N6O3	064124-21-6	30
4			Hexadecanal	240	C16H32O	000629-80-1	22
5			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
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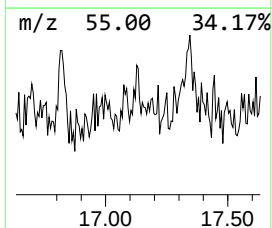
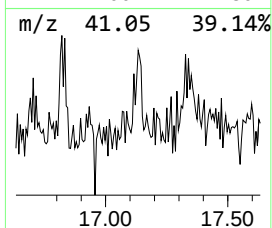
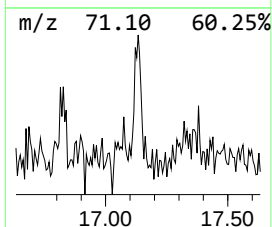
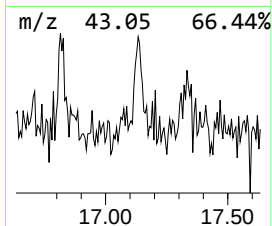
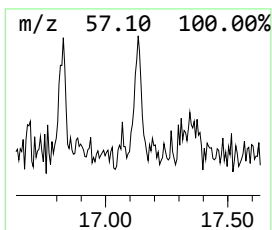
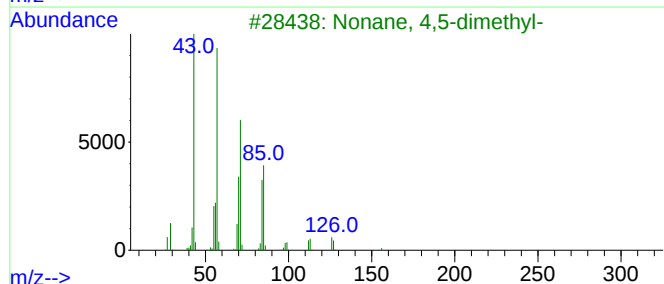
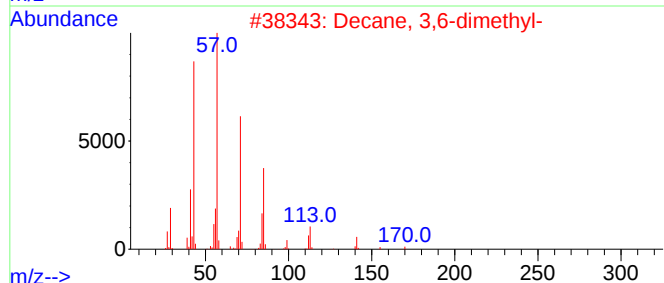
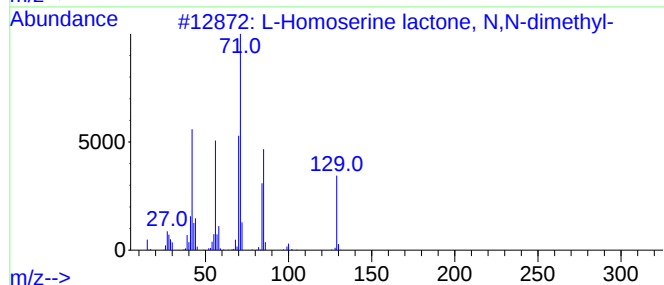
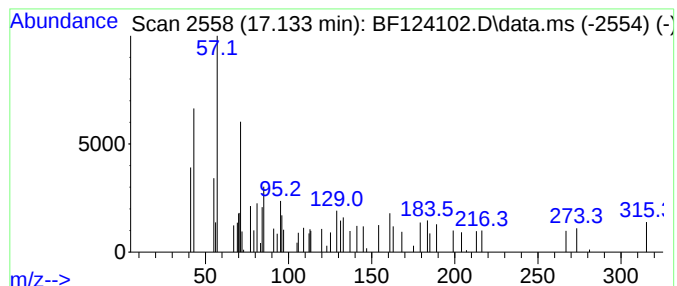
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown17.133 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.133	2.79 ng	46345	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Homoserine lactone, N,N-dimethyl-	129	C6H11NO2	1000374-45-7	46
2			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	35
3			Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	35
4			Undecane, 5-methyl-	170	C12H26	001632-70-8	35
5			Decane, 5-ethyl-5-methyl-	184	C13H28	017312-74-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

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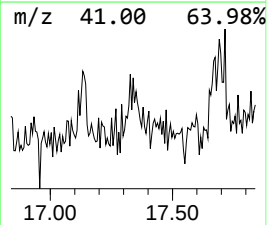
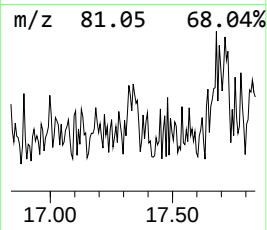
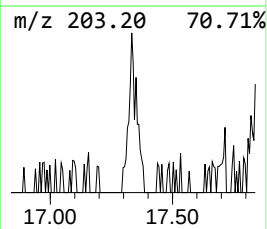
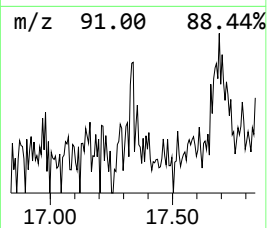
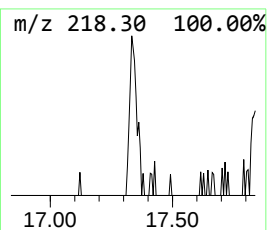
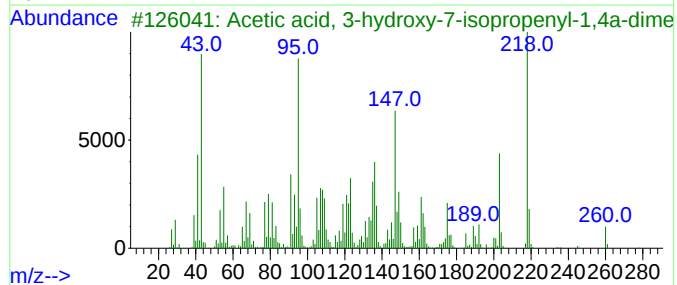
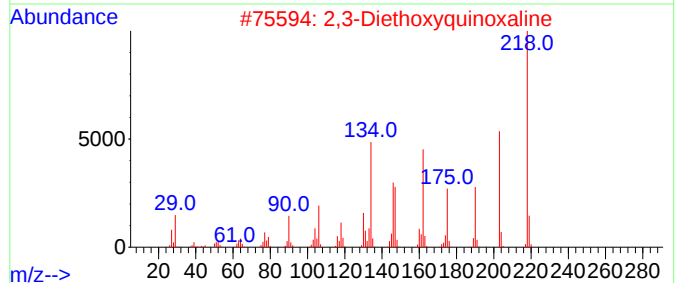
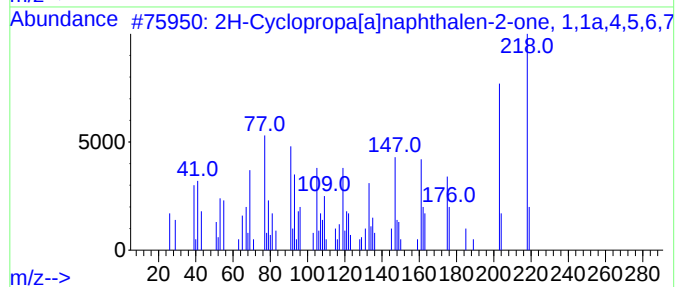
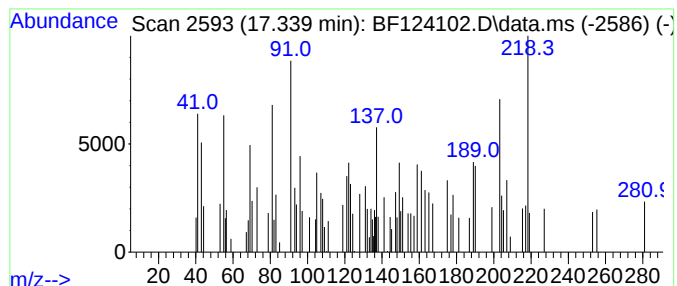
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown17.339 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.339	6.37 ng	105690	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	35
2			2,3-Diethoxyquinoxaline	218	C12H14N2O2	057050-66-5	30
3			Acetic acid, 3-hydroxy-7-isoprop...	278	C17H26O3	1000187-37-6	27
4			3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	22
5			7b-Phenyl-2a,7b-dihydro-3H-cyclo...	218	C17H14	138089-70-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
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ALS Vial : 15 Sample Multiplier: 1

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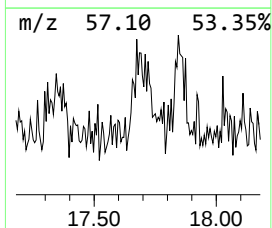
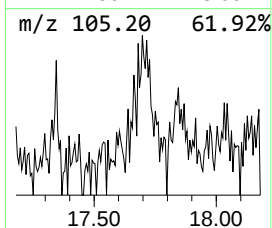
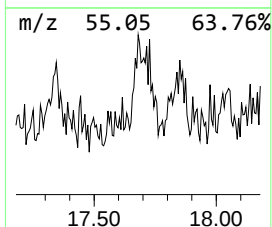
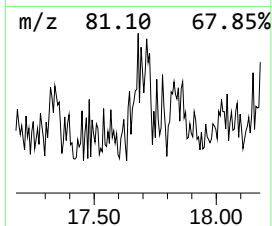
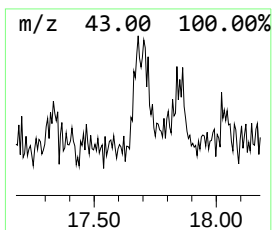
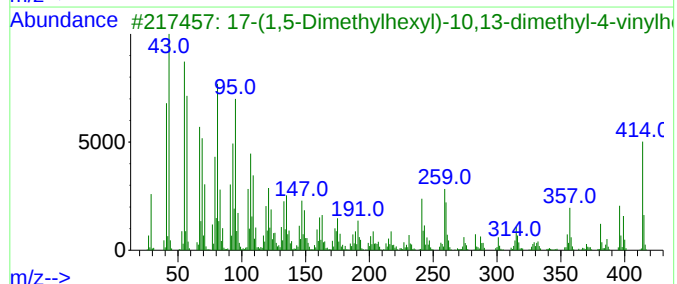
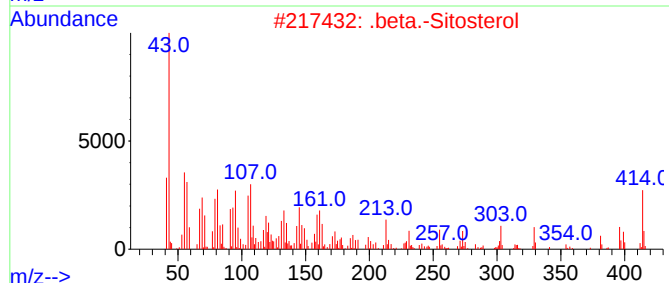
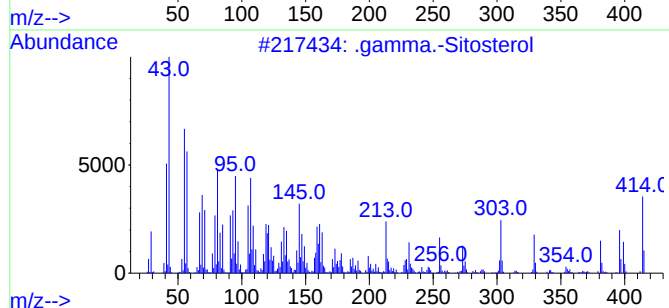
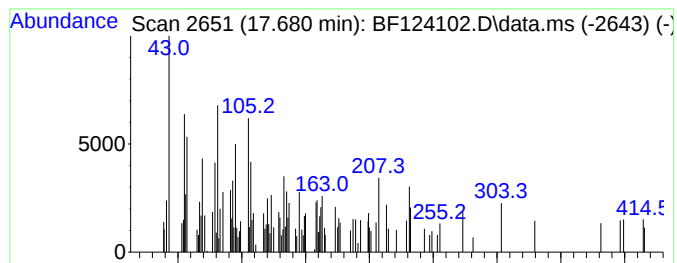
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 .gamma.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.680	7.68 ng	127365	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Sitosterol	414	C29H50O	000083-47-6	53
2			.beta.-Sitosterol	414	C29H50O	000083-46-5	47
3			17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	46
4			Dihydrosarsasapogenin-5,17(20)-dien	414	C27H42O3	096974-10-6	43
5			Germacra-1(10),4,11(13)-trien-12...	232	C15H20O2	000553-21-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
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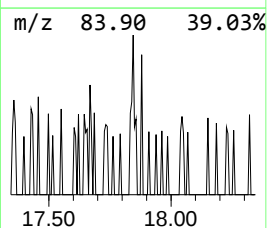
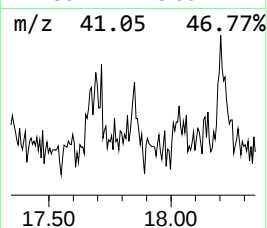
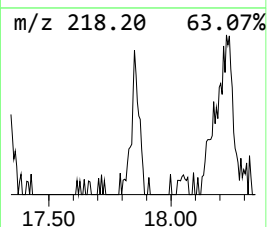
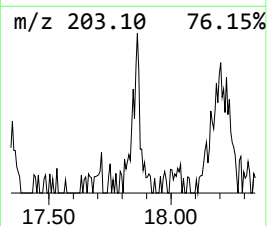
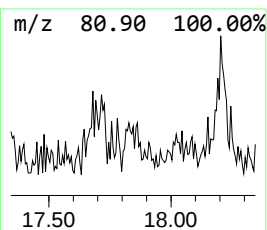
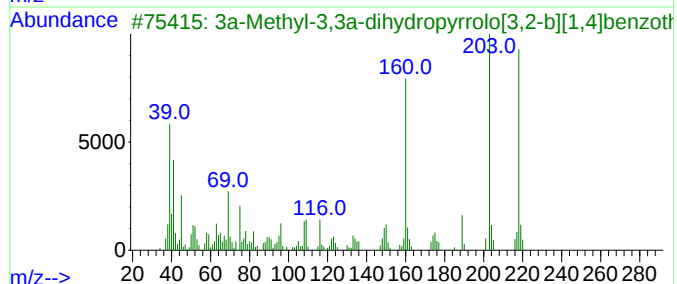
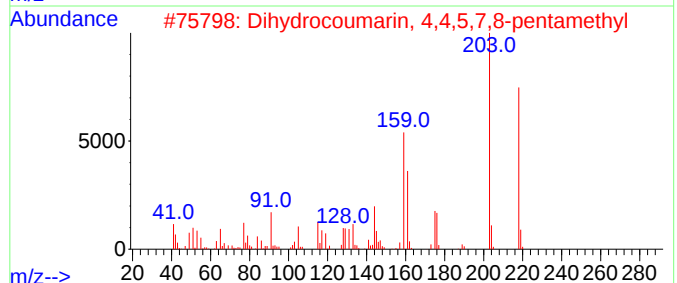
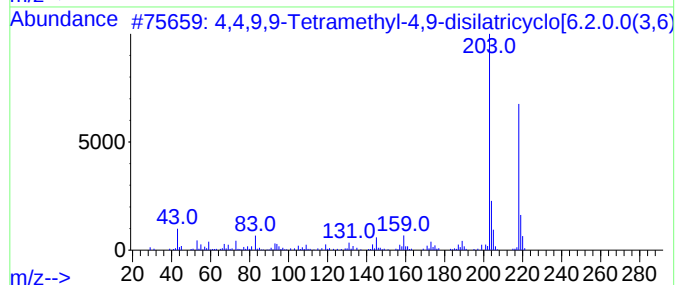
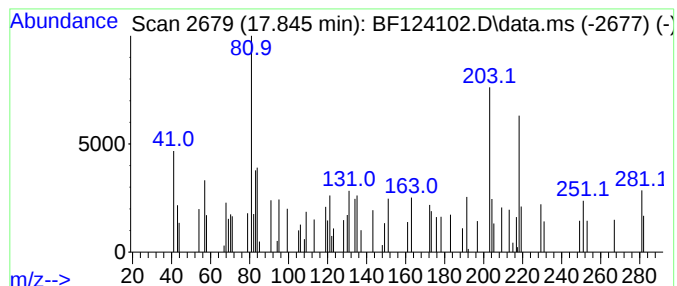
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 unknown17.845 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.845	5.30 ng	87972	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4,9,9-Tetramethyl-4,9-disilatr...	218	C12H18Si2	1000280-67-7	25		
2	Dihydrocoumarin, 4,4,5,7,8-penta...	218	C14H18O2	039170-97-3	22		
3	3a-Methyl-3,3a-dihydropyrrolo[3,...	218	C11H10N2OS	017163-68-7	12		
4	Acetamide, N-(3-methylphenyl)- 2...	203	C9H8F3NO	1000307-30-9	11		
5	[1,2,4]Triazolo[4,3-b][1,2,4]tri...	203	C8H5N5S	1000338-28-4	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
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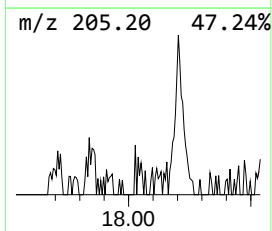
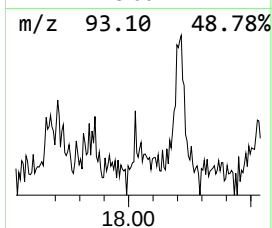
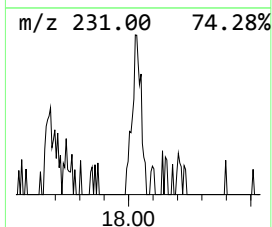
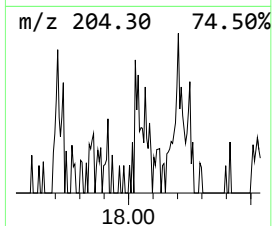
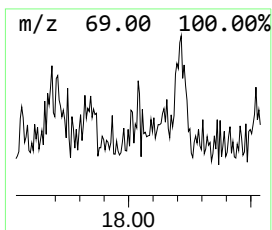
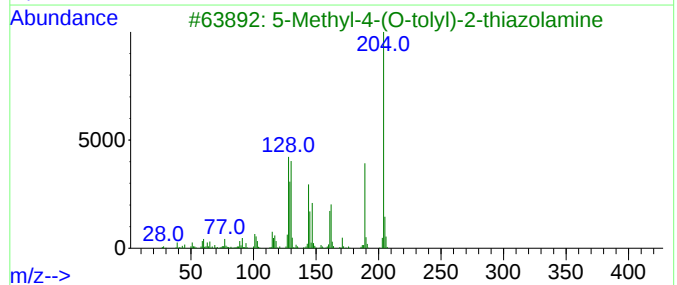
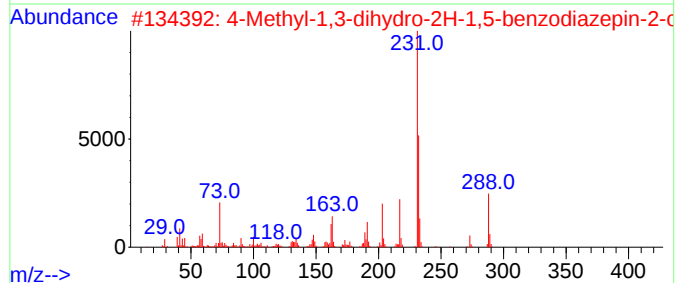
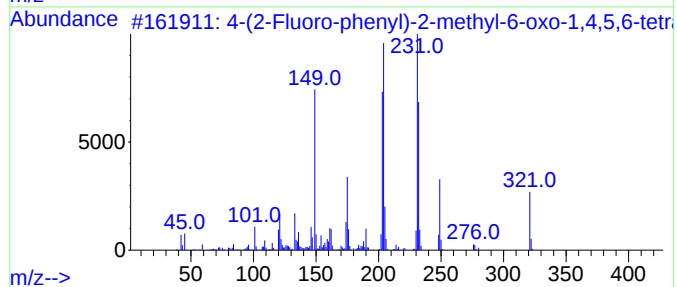
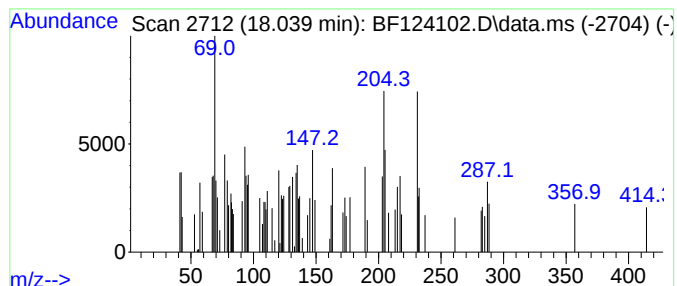
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 unknown18.039 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	5.25 ng	87052	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(2-Fluoro-phenyl)-2-methyl-6-o...	321	C17H20FN04	1000296-49-0	37		
2	4-Methyl-1,3-dihydro-2H-1,5-benz...	288	C16H24N2OSi	1000331-96-3	22		
3	5-Methyl-4-(O-tolyl)-2-thiazolamine	204	C11H12N2S	016942-68-0	22		
4	Phenol, 3,5-bis(1-pyrrolidinyl)-	232	C14H20N2O	016857-92-4	14		
5	Iron,(2-thenoyl)dicarbonyl-.pi.-...	288	C12H8FeO3S	059308-03-1	14		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-073

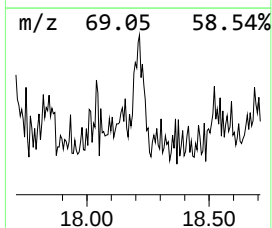
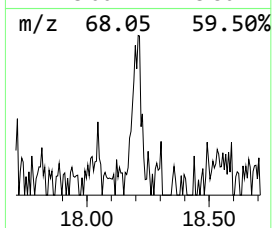
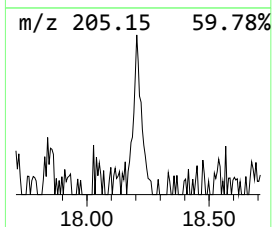
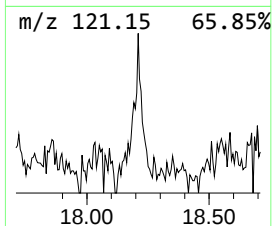
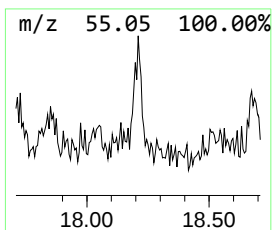
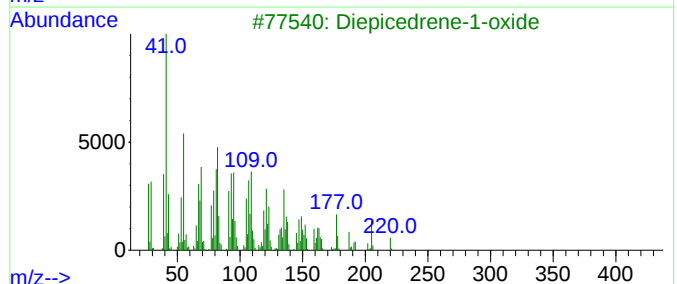
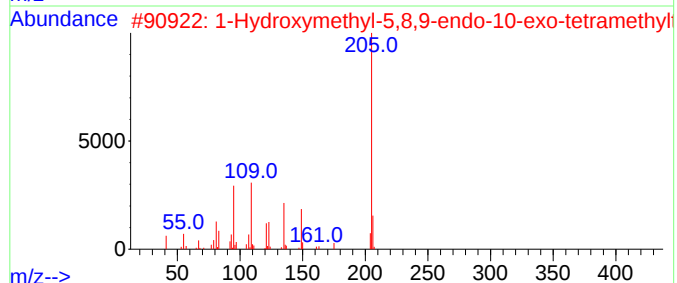
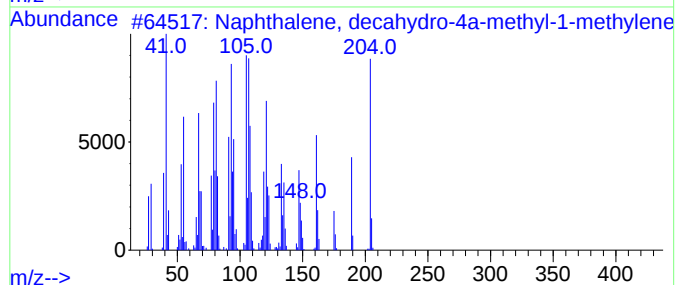
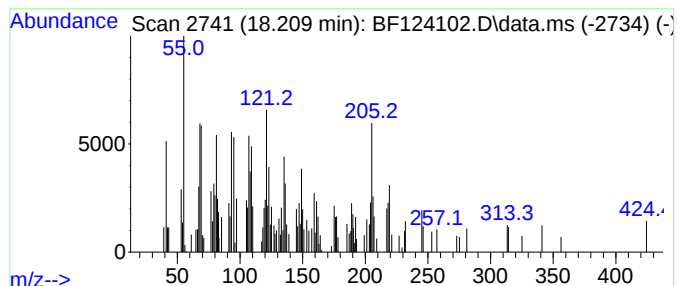
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Naphthalene, decahydro-4a-m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.209	17.72 ng	293917	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	56
2			1-Hydroxymethyl-5,8,9-endo-10-ex...	236	C16H28O	1000140-32-9	53
3			Diepicedrene-1-oxide	220	C15H24O	1000156-11-0	53
4			6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	18
5			Thioctic acid	206	C8H14O2S2	001077-28-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124102.D
Acq On : 27 May 2021 20:32
Operator : JU/CG
Sample : M2539-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-073

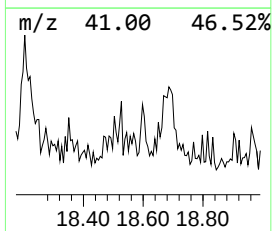
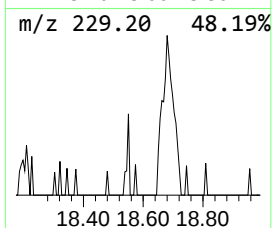
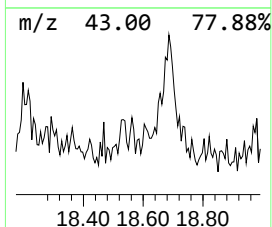
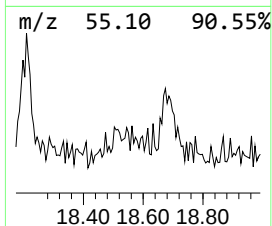
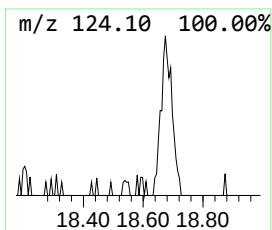
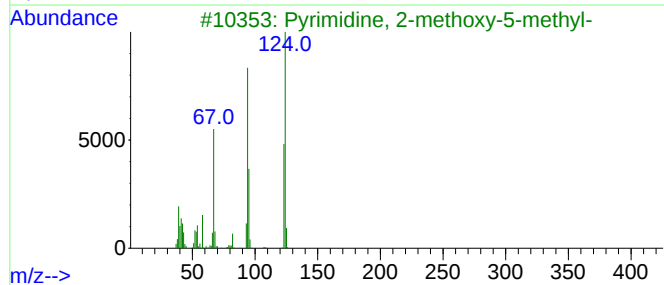
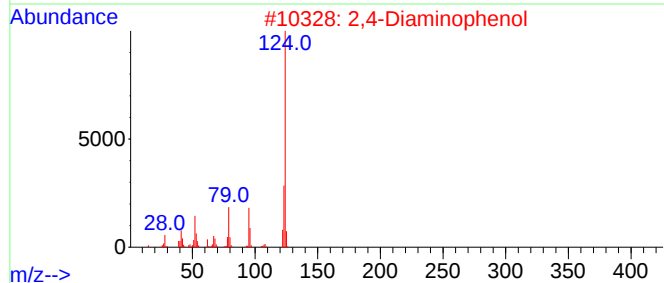
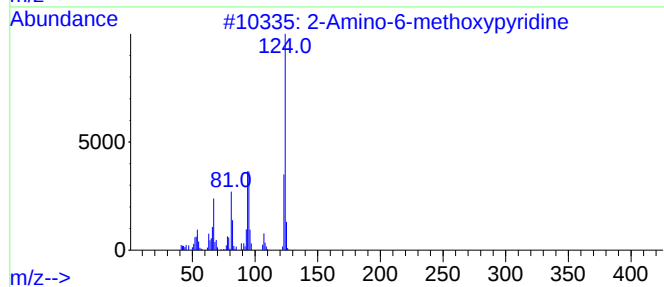
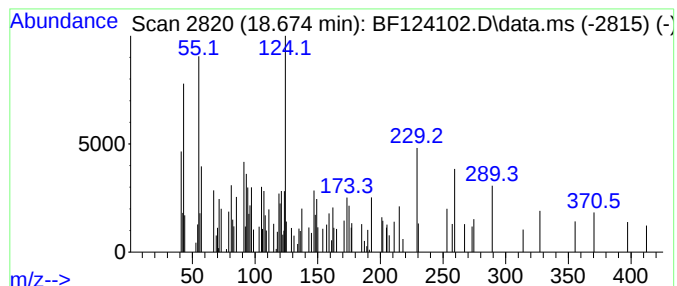
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 unknown18.674 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.674	5.52 ng	91488	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Amino-6-methoxypyridine	124	C6H8N2O	017920-35-3	30
2			2,4-Diaminophenol	124	C6H8N2O	000095-86-3	30
3			Pyrimidine, 2-methoxy-5-methyl-	124	C6H8N2O	017758-07-5	27
4			1,4-Benzenediol, 2-methyl-	124	C7H8O2	000095-71-6	27
5			1,3-Benzenediol, 2-methyl-	124	C7H8O2	000608-25-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
 Data File : BF124102.D
 Acq On : 27 May 2021 20:32
 Operator : JU/CG
 Sample : M2539-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-073

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.152	54.5	ng	702645	1	6.875	257691	20.0
Ethanol, 2-(2-b...	8.057	4.9	ng	77767	2	8.157	317637	20.0
unknown13.639	13.639	22.8	ng	357040	5	14.039	312959	20.0
Undecane, 5-eth...	13.886	3.2	ng	50353	5	14.039	312959	20.0
Benzoic acid, 2...	13.910	5.8	ng	90600	5	14.039	312959	20.0
Heptacosane	14.510	4.3	ng	67968	5	14.039	312959	20.0
unknown14.569	14.569	6.3	ng	98805	5	14.039	312959	20.0
Tetradecane	14.821	2.8	ng	45560	6	15.527	331686	20.0
Hentriacontane	15.169	8.1	ng	133952	6	15.527	331686	20.0
unknown15.762	15.762	3.0	ng	50038	6	15.527	331686	20.0
Tetratetracontane	16.004	6.6	ng	109744	6	15.527	331686	20.0
dl-.alpha.-Toco...	16.292	3.0	ng	50041	6	15.527	331686	20.0
unknown16.827	16.827	3.4	ng	57086	6	15.527	331686	20.0
unknown17.133	17.133	2.8	ng	46345	6	15.527	331686	20.0
unknown17.339	17.339	6.4	ng	105690	6	15.527	331686	20.0
.gamma.-Sitosterol	17.680	7.7	ng	127365	6	15.527	331686	20.0
unknown17.845	17.845	5.3	ng	87972	6	15.527	331686	20.0
unknown18.039	18.039	5.3	ng	87052	6	15.527	331686	20.0
Naphthalene, de...	18.209	17.7	ng	293917	6	15.527	331686	20.0
unknown18.674	18.674	5.5	ng	91488	6	15.527	331686	20.0