

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
 Data File : BF133495.D
 Acq On : 25 May 2023 19:03
 Operator : CG\JU
 Sample : 02908-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB10A

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	11	15	26	rVB3	45048	74484	4.28%	0.534%
2	4.193	352	358	369	rBV3	24995	53004	3.04%	0.380%
3	5.034	497	501	506	rVB	111535	126072	7.24%	0.904%
4	5.440	565	570	573	rBV	1924271	1741201	100.00%	12.485%
5	6.452	737	742	745	rBV	1902673	1669141	95.86%	11.968%
6	6.834	804	807	811	rVB	771586	570204	32.75%	4.089%
7	7.393	898	902	905	rBV	1200210	1028466	59.07%	7.375%
8	8.116	1022	1025	1029	rBV	852802	673716	38.69%	4.831%
9	8.693	1119	1123	1126	rBV2	16807	23669	1.36%	0.170%
10	8.963	1166	1169	1176	rVB2	45852	48964	2.81%	0.351%
11	9.193	1205	1208	1212	rVB	1972975	1611465	92.55%	11.555%
12	9.875	1320	1324	1327	rVB	717445	600506	34.49%	4.306%
13	10.528	1432	1435	1438	rBV	30179	20984	1.21%	0.150%
14	10.587	1440	1445	1448	rBV	158283	121167	6.96%	0.869%
15	10.657	1453	1457	1460	rBV	1119821	886076	50.89%	6.354%
16	11.357	1573	1576	1579	rBV	717473	571965	32.85%	4.101%
17	11.886	1662	1666	1671	rBV	104133	103587	5.95%	0.743%
18	12.569	1779	1782	1785	rBV	85015	76136	4.37%	0.546%
19	12.675	1796	1800	1805	rBV2	32678	37666	2.16%	0.270%
20	12.798	1814	1821	1824	rBV	88828	84992	4.88%	0.609%
21	12.945	1843	1846	1850	rVB	1495834	1372177	78.81%	9.839%
22	13.192	1881	1888	1891	rBV6	11257	18930	1.09%	0.136%
23	13.857	1996	2001	2010	rBV3	75471	114149	6.56%	0.818%
24	13.998	2021	2025	2028	rBV	779633	720300	41.37%	5.165%
25	14.022	2028	2029	2035	rVB	50445	43699	2.51%	0.313%
26	14.104	2039	2043	2047	rVB5	27287	34263	1.97%	0.246%
27	14.486	2104	2108	2114	rBV6	26047	51525	2.96%	0.369%
28	14.874	2170	2174	2181	rVB5	20263	36274	2.08%	0.260%
29	15.033	2197	2201	2204	rBV	61272	91880	5.28%	0.659%
30	15.133	2214	2218	2222	rBV4	27919	32910	1.89%	0.236%
31	15.333	2249	2252	2258	rVB	41773	54866	3.15%	0.393%
32	15.392	2258	2262	2268	rBV	62172	80057	4.60%	0.574%
33	15.463	2268	2274	2278	rBV	584789	747772	42.95%	5.362%
34	15.757	2319	2324	2331	rBV2	96885	152443	8.76%	1.093%
35	15.951	2354	2357	2361	rVB3	20516	24975	1.43%	0.179%
36	16.010	2362	2367	2374	rVB9	17521	36366	2.09%	0.261%

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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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.904	2514	2519	2525	rBV3	25972	50718	2.91%	0.364%
38	17.339	2589	2593	2598	rVB2	23815	41877	2.41%	0.300%
39	17.521	2619	2624	2637	rBV8	39323	117485	6.75%	0.842%

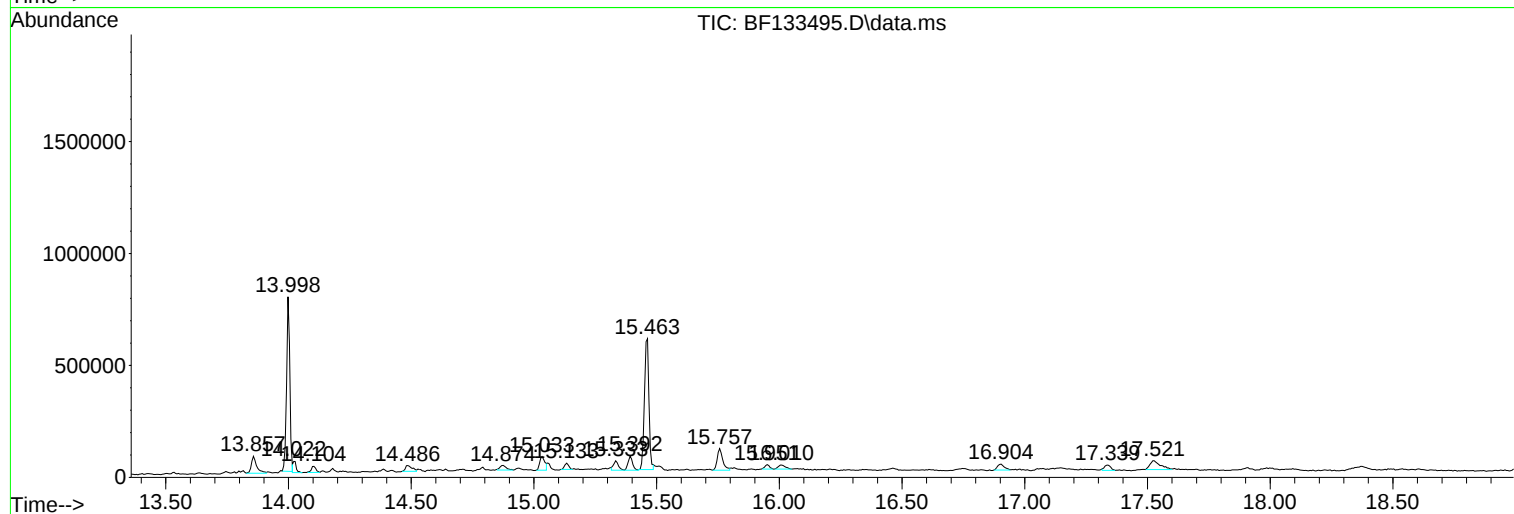
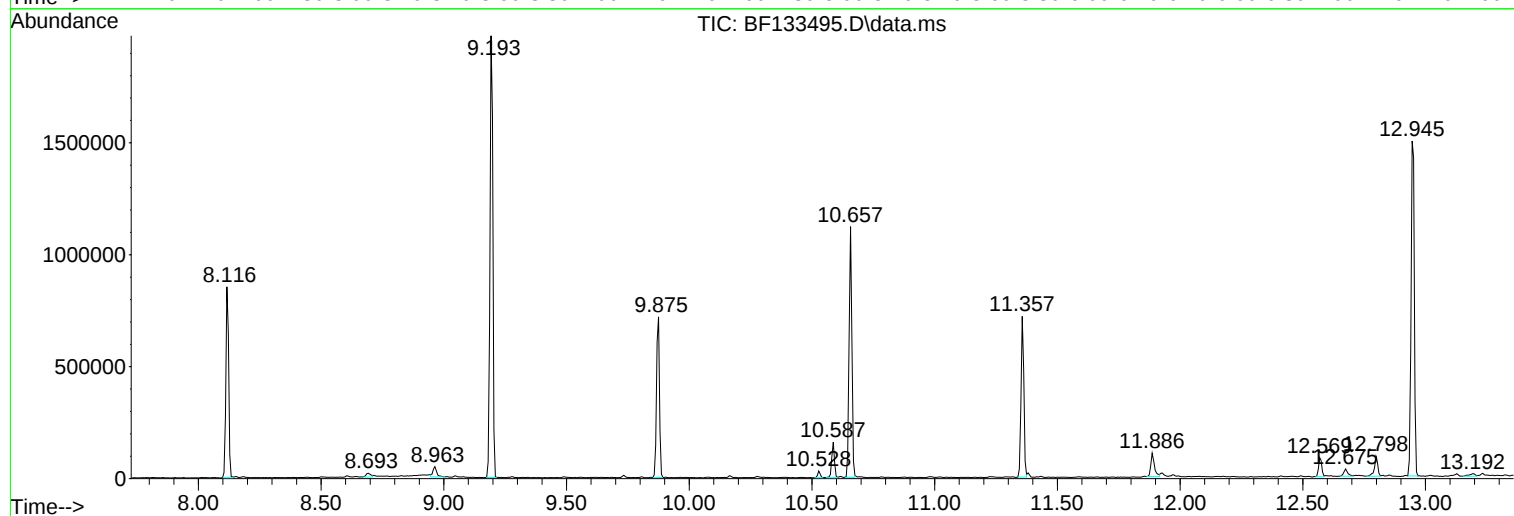
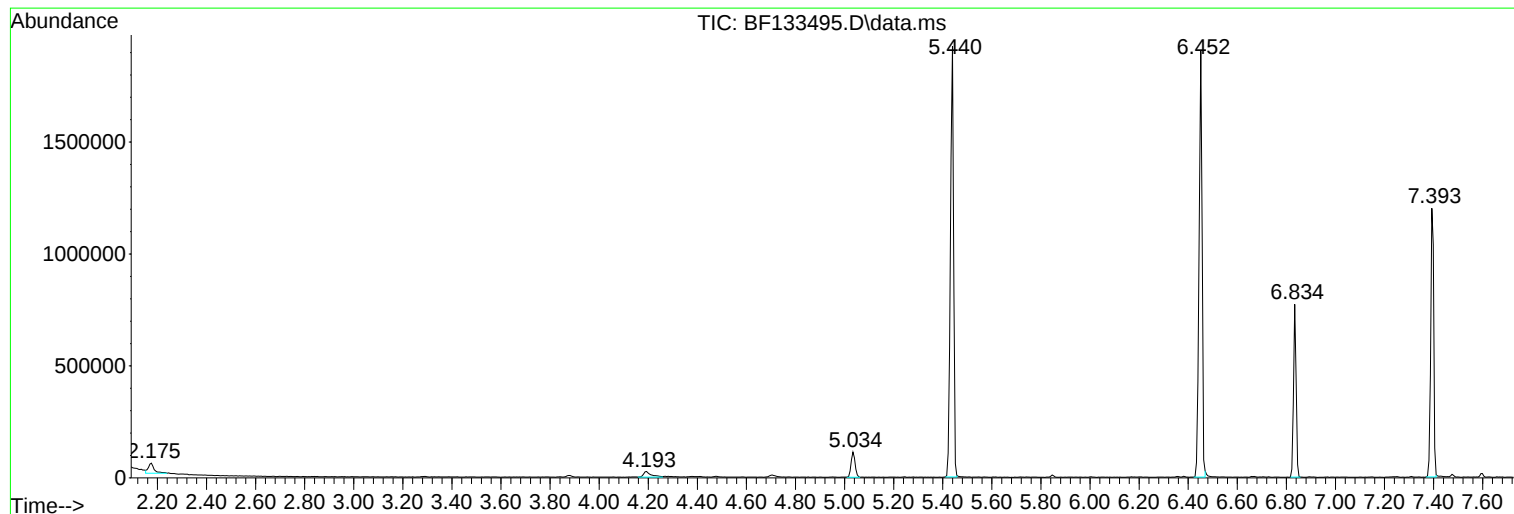
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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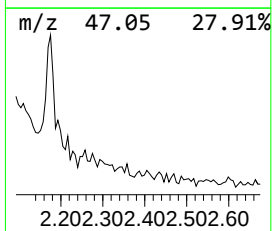
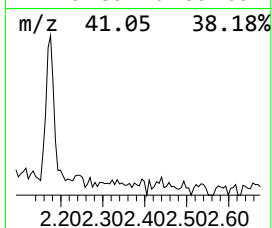
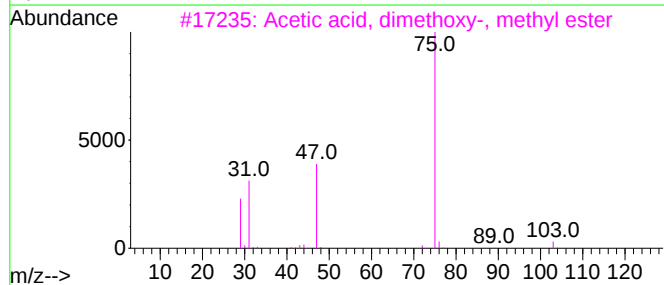
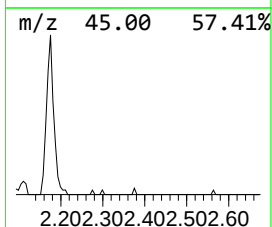
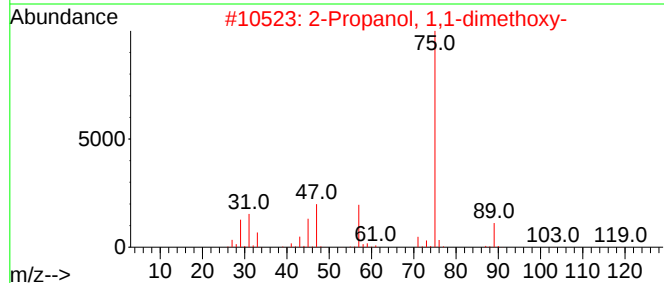
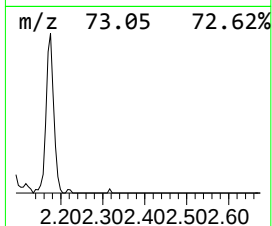
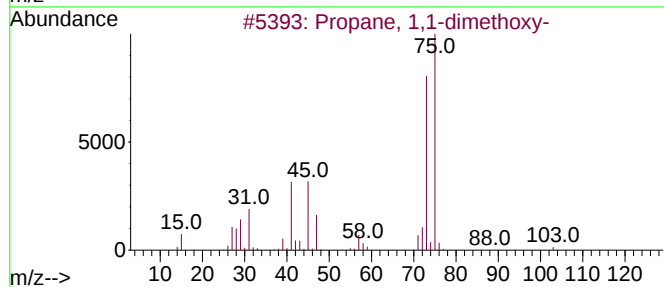
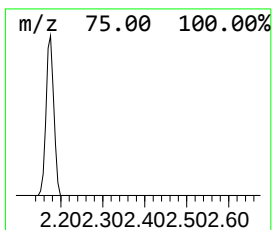
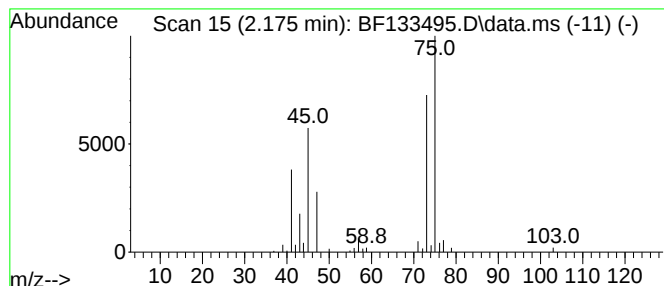
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	2.61 ng	74484	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36
3			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	28
4			2-Propanol, 1,3-dimethoxy-	120	C5H12O3	000623-69-8	12
5			2-Hexanol, 5-methyl-	116	C7H16O	000627-59-8	9



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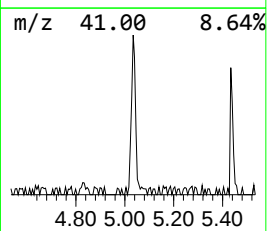
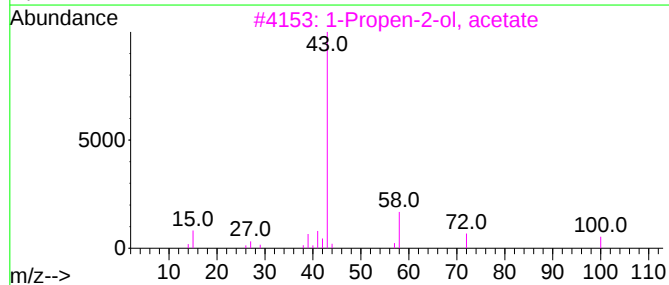
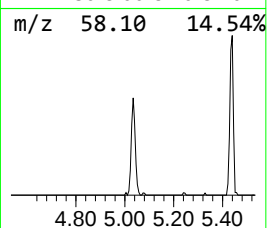
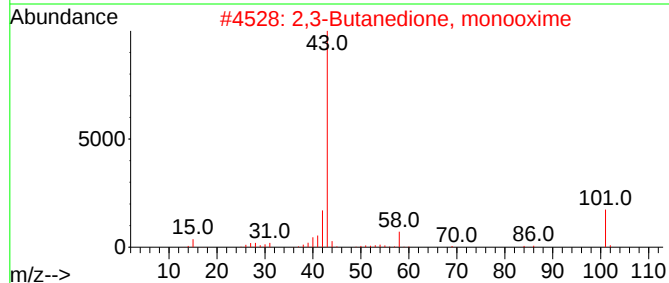
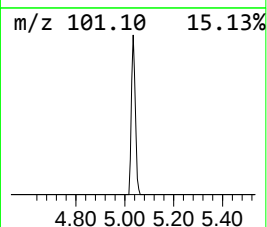
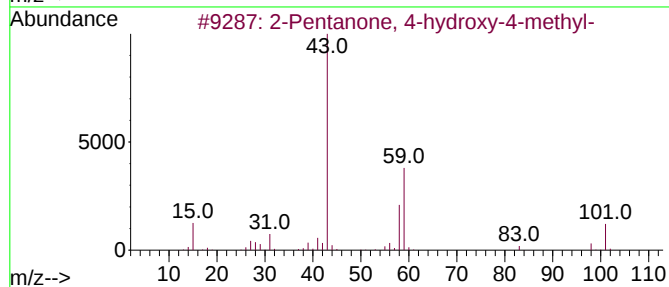
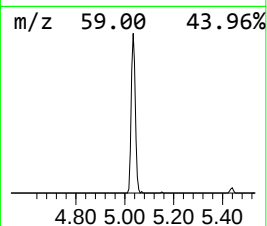
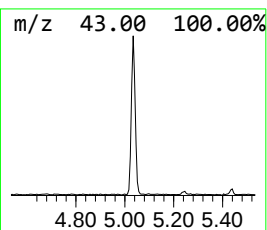
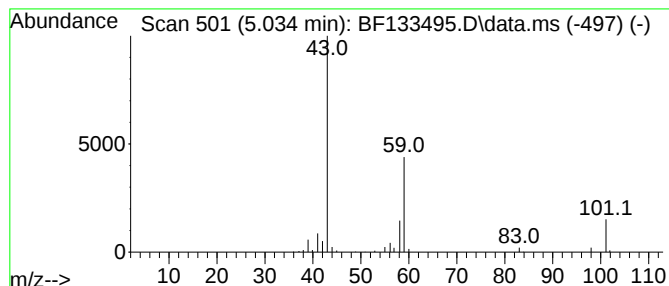
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	4.42 ng	126072	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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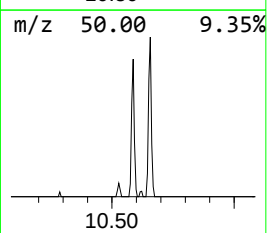
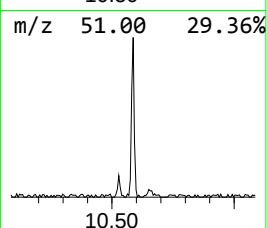
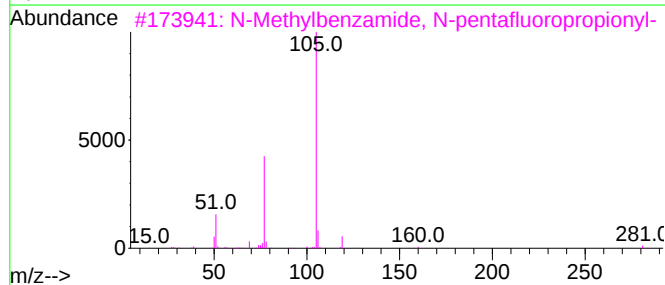
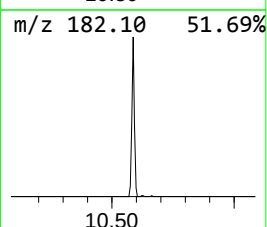
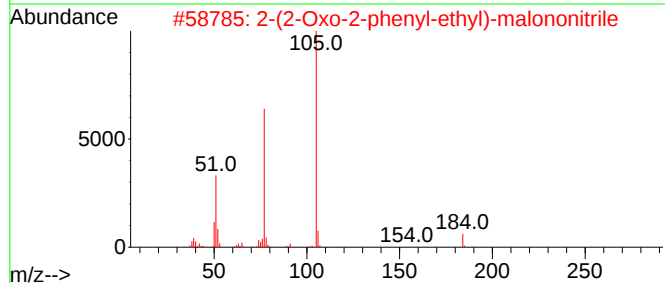
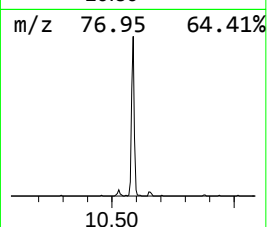
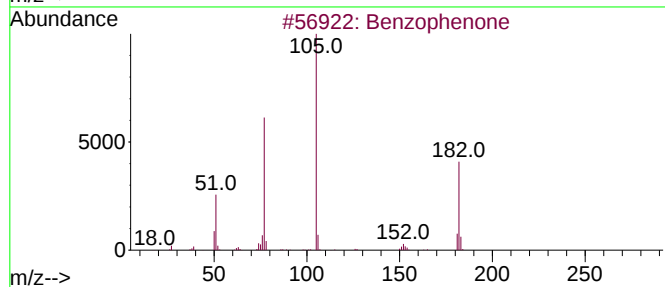
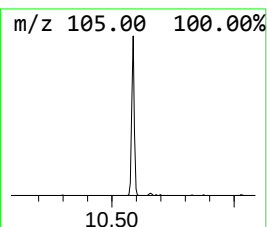
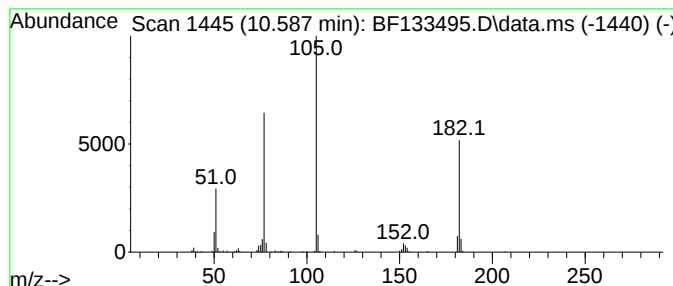
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	4.04 ng	121167	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	58
3			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50
5			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	50



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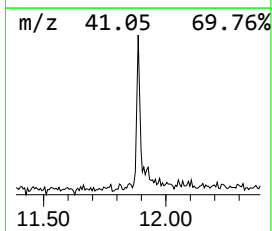
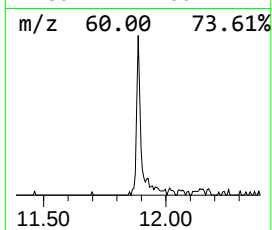
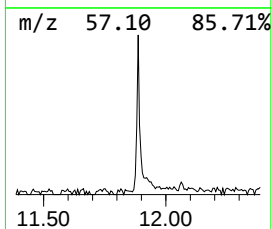
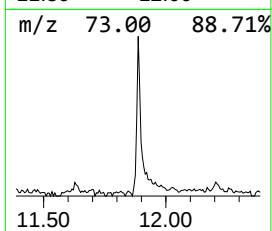
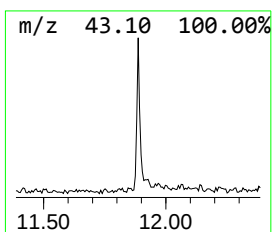
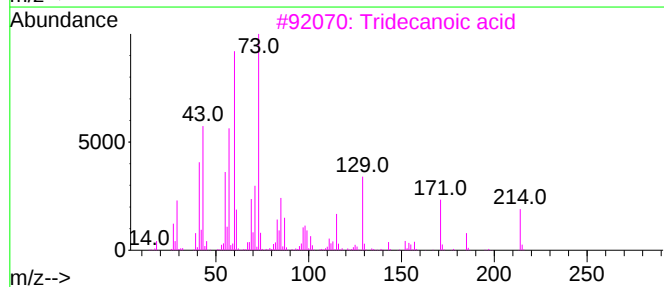
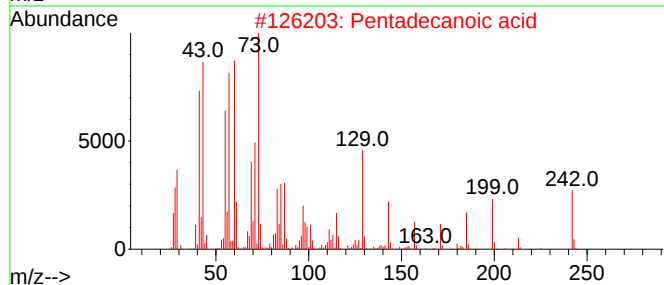
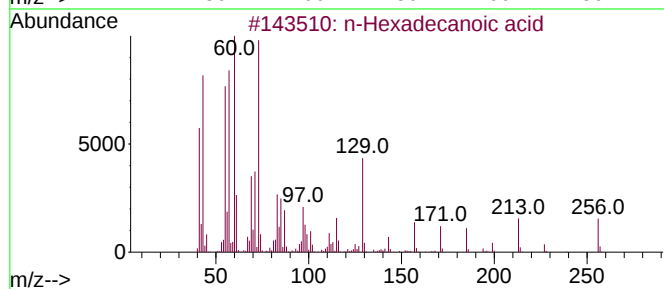
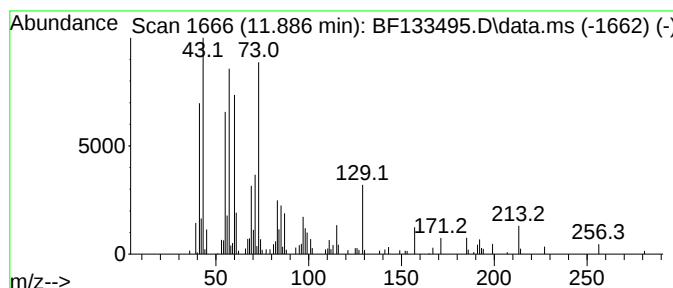
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.887	3.62 ng	103587	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	78
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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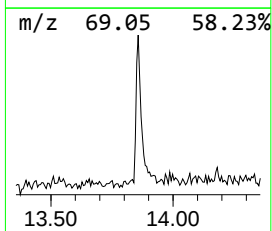
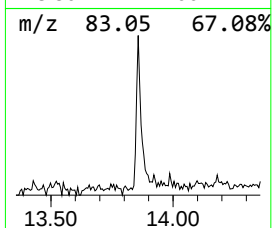
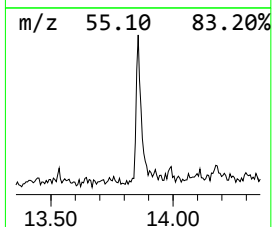
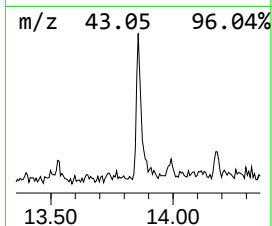
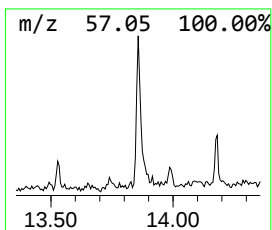
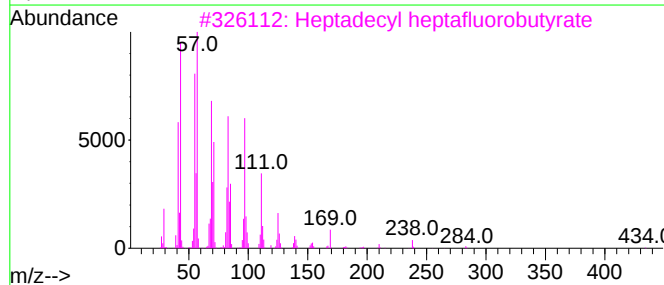
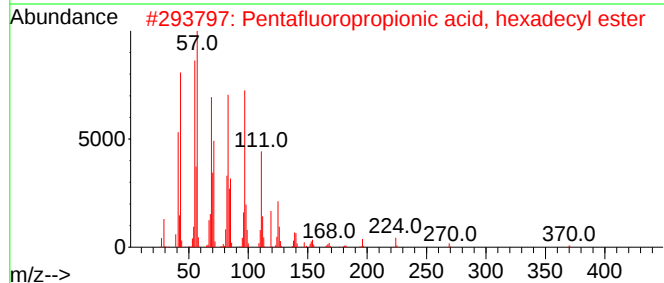
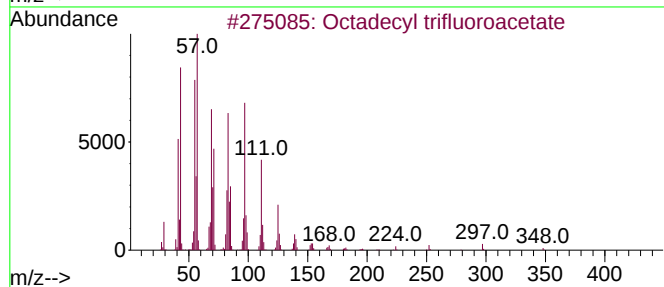
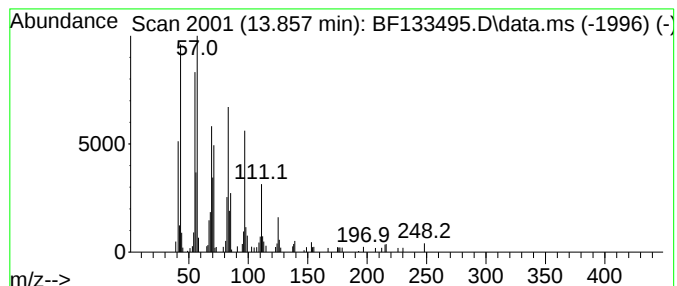
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	3.17 ng	114149	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
2			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5			Heptafluorobutyric acid, pentadecyl ester	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133495.D
Acq On : 25 May 2023 19:03
Operator : CG\JU
Sample : 02908-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB10A

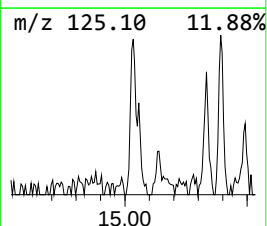
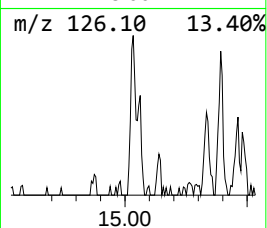
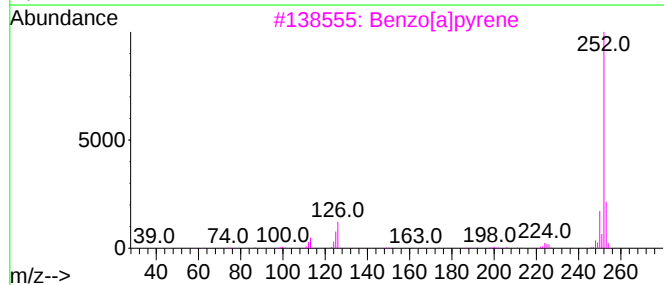
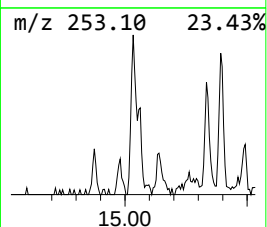
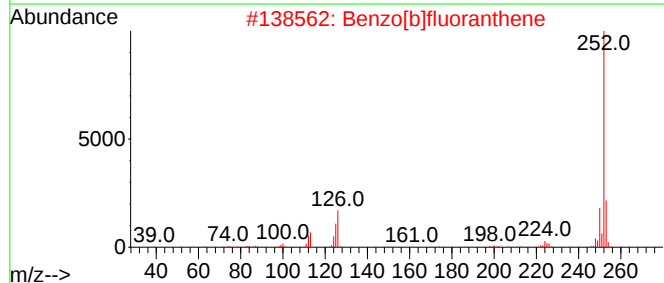
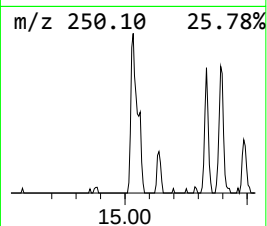
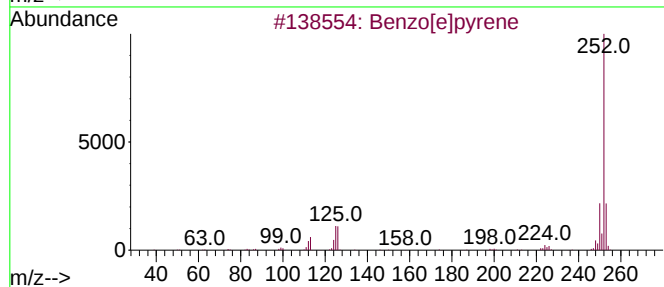
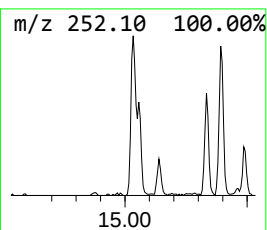
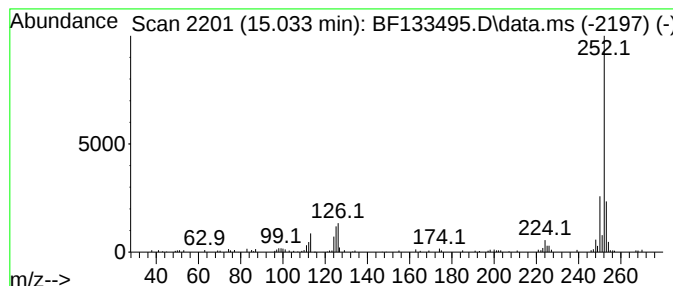
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.033	2.46 ng	91880	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
3			Benzo[a]pyrene	252	C20H12	000050-32-8	95
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5			Perylene	252	C20H12	000198-55-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133495.D
Acq On : 25 May 2023 19:03
Operator : CG\JU
Sample : 02908-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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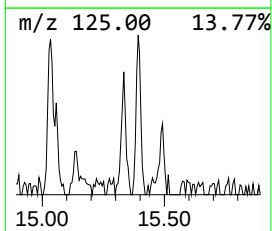
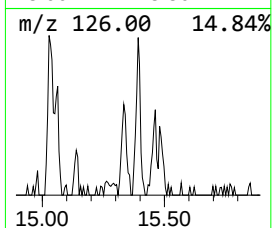
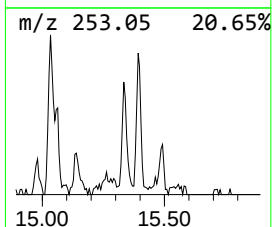
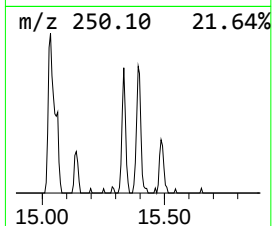
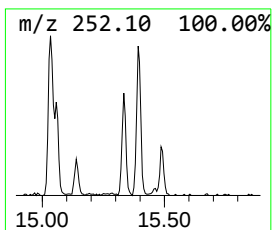
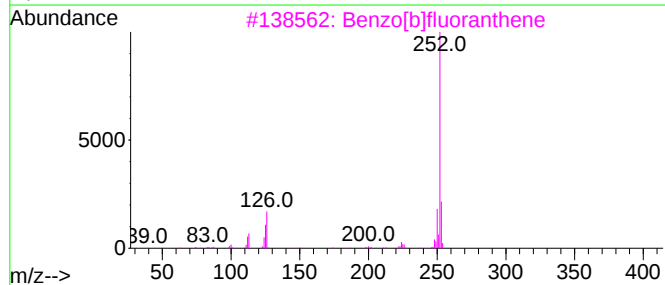
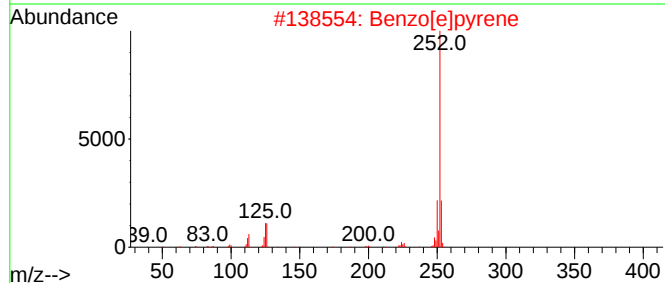
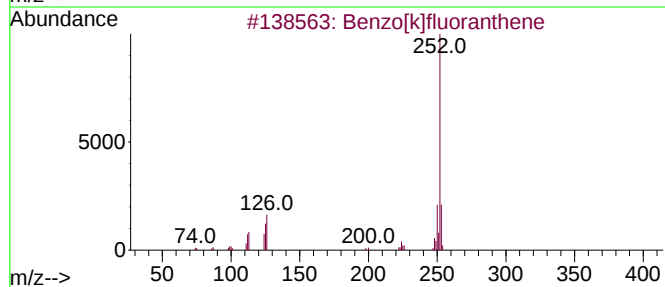
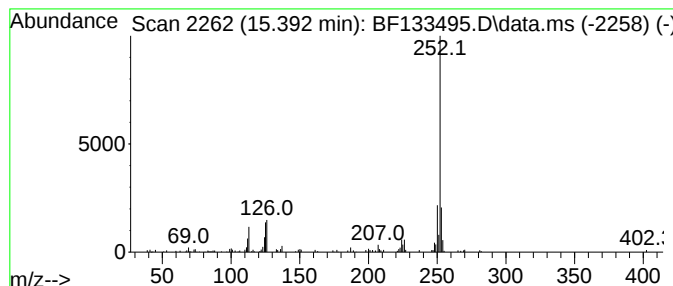
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[j]fluoranthene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	2.14 ng	80057	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
2			Benzo[e]pyrene	252	C20H12	000192-97-2	96
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
5			Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133495.D
Acq On : 25 May 2023 19:03
Operator : CG\JU
Sample : 02908-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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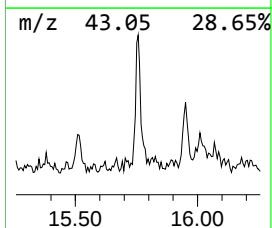
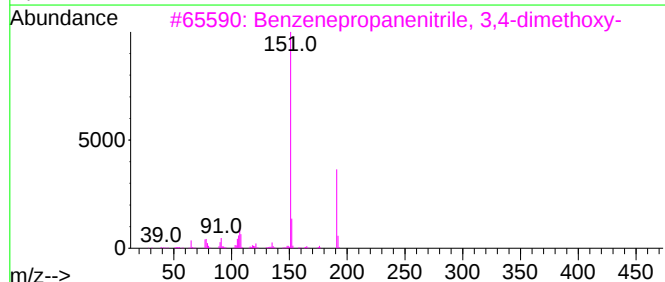
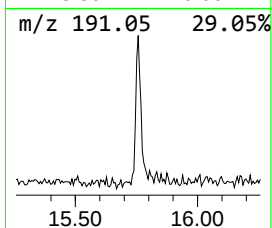
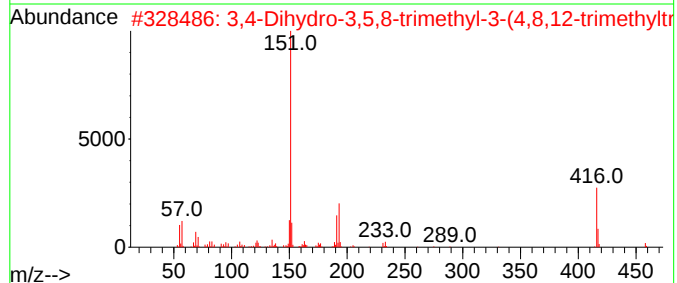
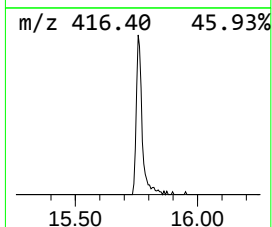
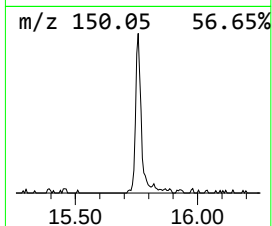
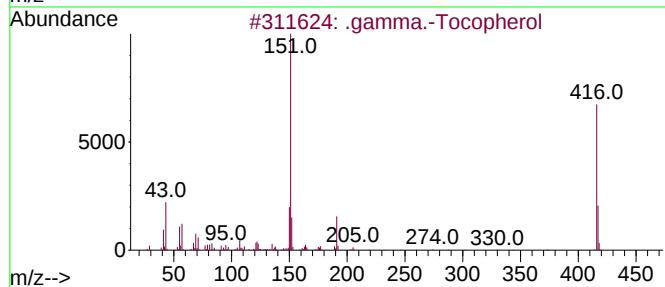
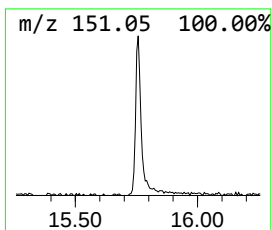
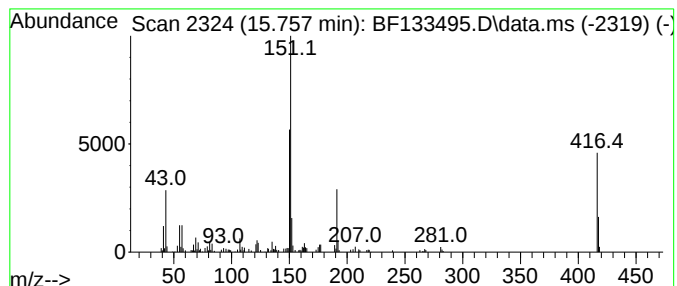
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 .gamma.-Tocopherol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.757	4.08 ng	152443	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Tocopherol	416	C28H48O2	007616-22-0	95
2			3,4-Dihydro-3,5,8-trimethyl-3-(4...	458	C30H50O3	1000105-71-9	52
3			Benzenepropanenitrile, 3,4-dimet...	191	C11H13NO2	049621-56-9	46
4			(1R,3R,3aS,4S,7R,9aR,10aR,Z)-7-I...	364	C23H40O3	1000495-80-5	38
5			3-(2,4-Dimethoxy-phenyl)-2-formy...	281	C14H19NO5	1000190-90-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133495.D
Acq On : 25 May 2023 19:03
Operator : CG\JU
Sample : 02908-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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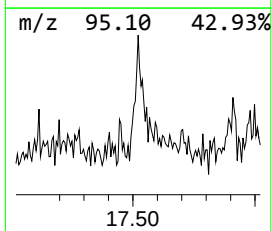
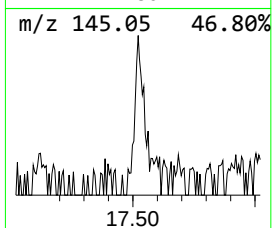
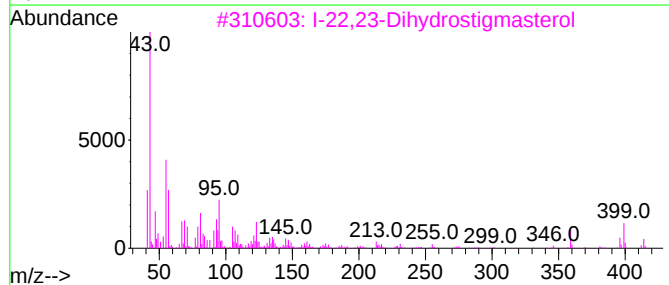
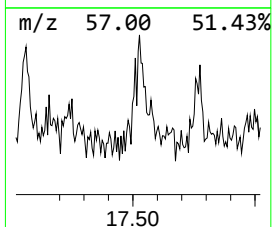
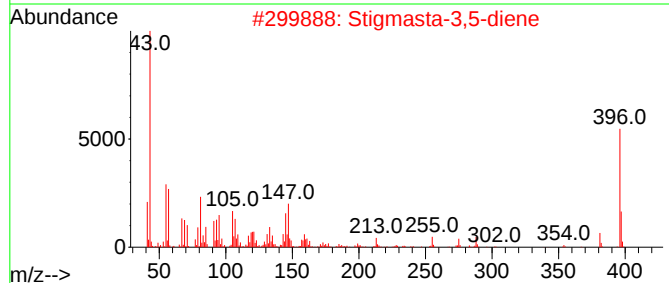
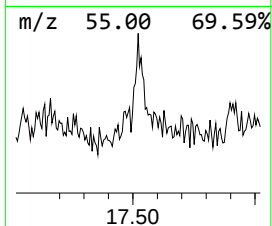
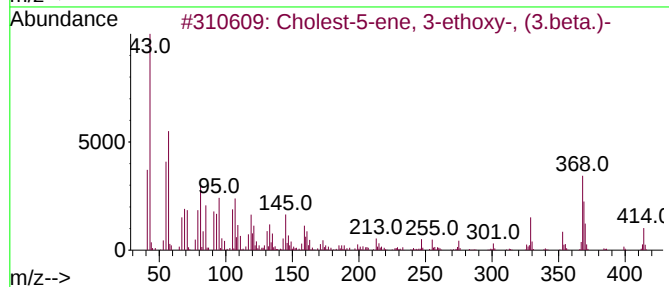
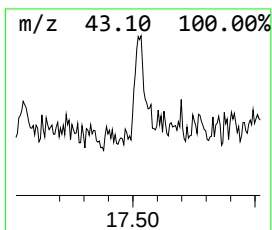
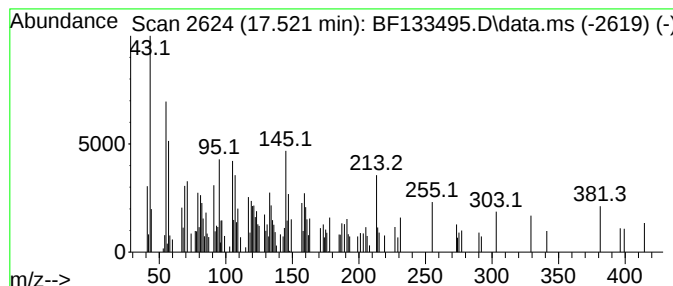
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.521 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.521	3.14 ng	117485	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	30
2			Stigmasta-3,5-diene	396	C29H48	004970-37-0	25
3			I-22,23-Dihydrostigmasterol	414	C29H50O	1000214-82-6	22
4			.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	12
5			Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052523\
Data File : BF133495.D
Acq On : 25 May 2023 19:03
Operator : CG\JU
Sample : 02908-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-di...	2.175	2.6	ng	74484	1	6.834	570204	20.0
2-Pentanone, 4-...	5.034	4.4	ng	126072	1	6.834	570204	20.0
Benzophenone	10.586	4.0	ng	121167	3	9.875	600506	20.0
n-Hexadecanoic ...	11.887	3.6	ng	103587	4	11.357	571965	20.0
Octadecyl trifl...	13.857	3.2	ng	114149	5	13.998	720300	20.0
Benzo[e]pyrene	15.033	2.5	ng	91880	6	15.463	747772	20.0
Benzo[j]fluoran...	15.392	2.1	ng	80057	6	15.463	747772	20.0
.gamma.-Tocopherol	15.757	4.1	ng	152443	6	15.463	747772	20.0
unknown17.521	17.521	3.1	ng	117485	6	15.463	747772	20.0