

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
 Data File : BF123496.D
 Acq On : 26 Mar 2021 20:35
 Operator : JU/CG
 Sample : M1792-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-5

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-BF032321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123496.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	20	29	35	rVB	1311013	1663485	28.67%	3.495%
2	2.363	39	47	56	rVB	281397	351923	6.06%	0.739%
3	3.469	231	235	251	rBV2	34698	87156	1.50%	0.183%
4	5.134	515	518	524	rVB	153969	188626	3.25%	0.396%
5	5.528	579	585	588	rBV	5541417	5491111	94.63%	11.536%
6	6.528	749	755	759	rBV	4938805	5802591	100.00%	12.191%
7	6.722	785	788	793	rBV	136703	121885	2.10%	0.256%
8	6.898	814	818	821	rBV	1981611	1581221	27.25%	3.322%
9	7.463	907	914	917	rBV	3407675	3693983	63.66%	7.761%
10	8.180	1031	1036	1040	rBV	2157118	2050533	35.34%	4.308%
11	9.263	1214	1220	1223	rBV	5777594	5043080	86.91%	10.595%
12	9.651	1282	1286	1290	rBV	521229	385523	6.64%	0.810%
13	9.945	1330	1336	1339	rBV	2530239	2273188	39.18%	4.776%
14	10.733	1464	1470	1473	rBV	4052392	3740168	64.46%	7.858%
15	11.098	1526	1532	1536	rBV2	129494	136890	2.36%	0.288%
16	11.433	1583	1589	1592	rBV	2531721	2139072	36.86%	4.494%
17	11.957	1674	1678	1688	rBV	678495	649000	11.18%	1.364%
18	13.021	1855	1859	1862	rBV	4062870	3445670	59.38%	7.239%
19	13.257	1894	1899	1903	rBV2	44949	72055	1.24%	0.151%
20	13.874	1998	2004	2007	rBV	78800	122214	2.11%	0.257%
21	13.927	2007	2013	2023	rBV3	548781	1194045	20.58%	2.509%
22	14.062	2032	2036	2037	rBV	1733909	1534172	26.44%	3.223%
23	14.368	2085	2088	2089	rBV	79998	61751	1.06%	0.130%
24	14.398	2089	2093	2096	rVB	3501083	3081997	53.11%	6.475%
25	14.574	2121	2123	2127	rVB	65802	75052	1.29%	0.158%
26	14.951	2184	2187	2191	rVB	104745	102981	1.77%	0.216%
27	15.221	2230	2233	2237	rVB	97795	101533	1.75%	0.213%
28	15.574	2288	2293	2298	rBV	1040249	1304044	22.47%	2.740%
29	16.080	2374	2379	2384	rVB2	65092	104640	1.80%	0.220%
30	16.145	2385	2390	2398	rBV5	86589	247324	4.26%	0.520%
31	16.903	2515	2519	2527	rVB3	74736	127065	2.19%	0.267%
32	17.315	2582	2589	2590	rBV6	69559	121161	2.09%	0.255%
33	17.739	2655	2661	2668	rBV6	69477	206926	3.57%	0.435%
34	18.086	2714	2720	2735	rVB6	77372	295703	5.10%	0.621%

Sum of corrected areas: 47597768

Instrument :

BNA_F

ClientSampleId :

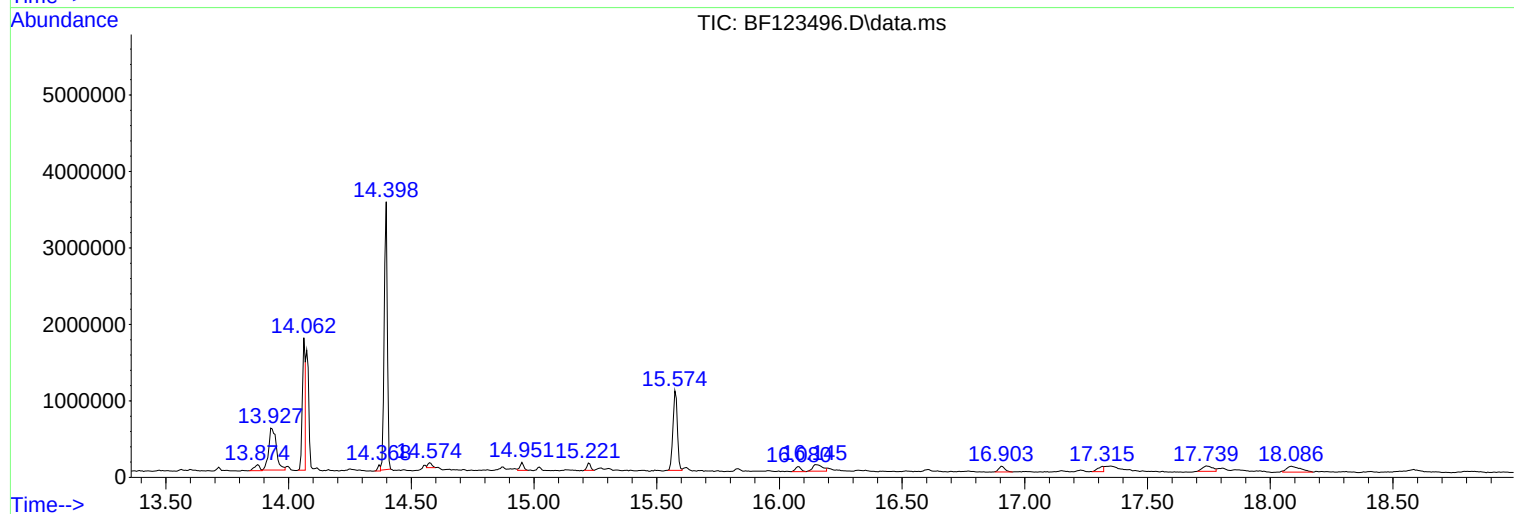
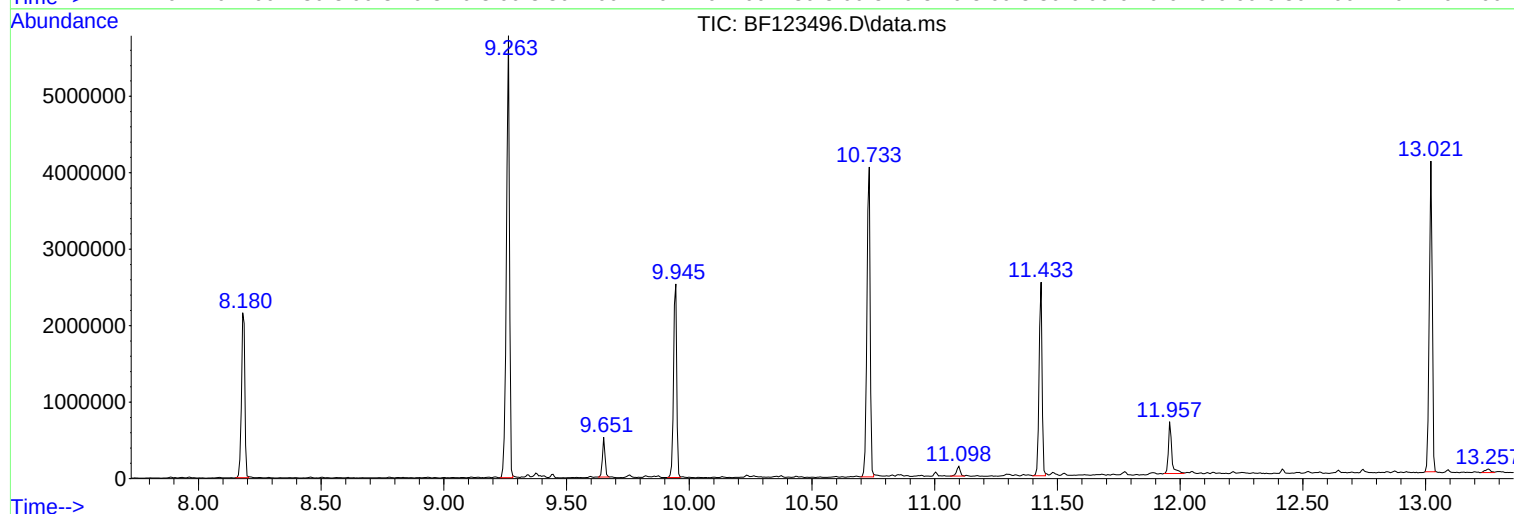
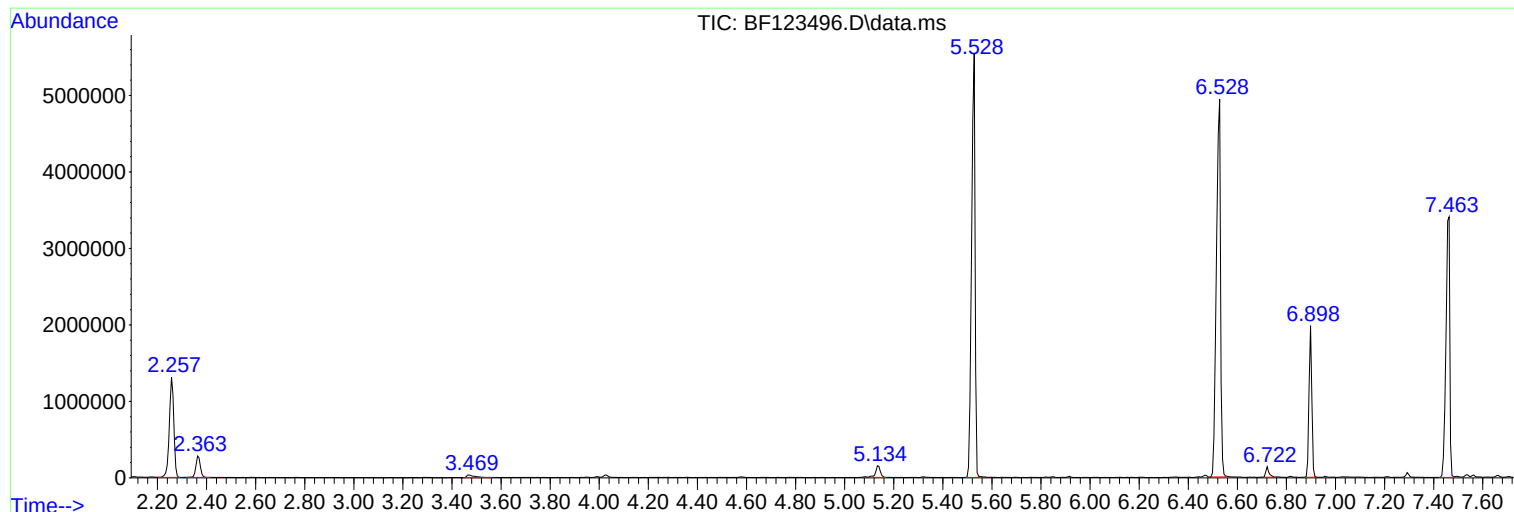
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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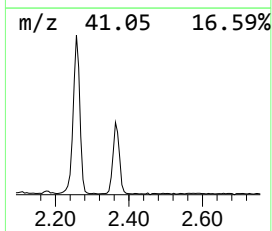
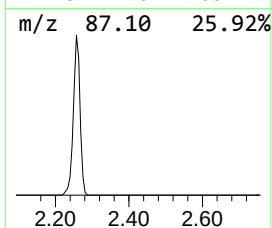
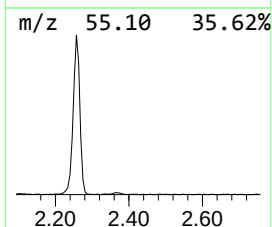
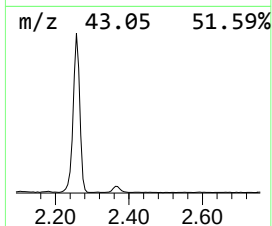
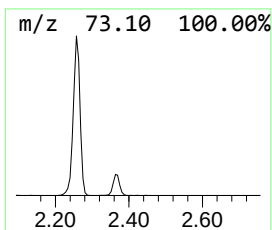
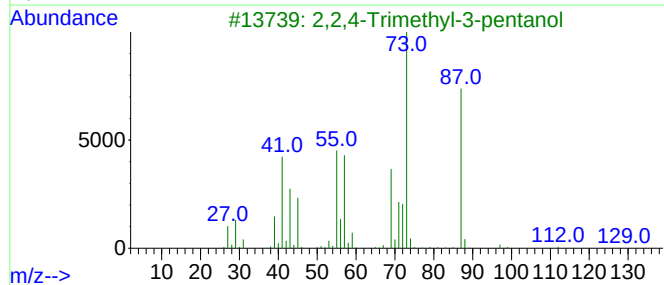
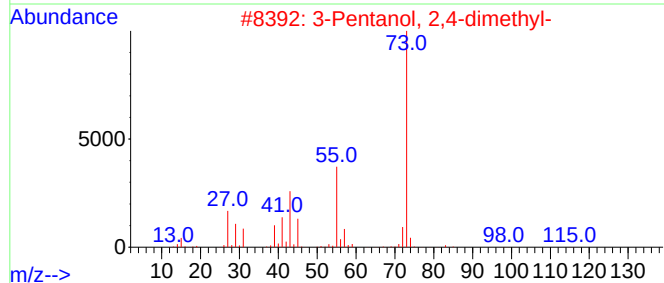
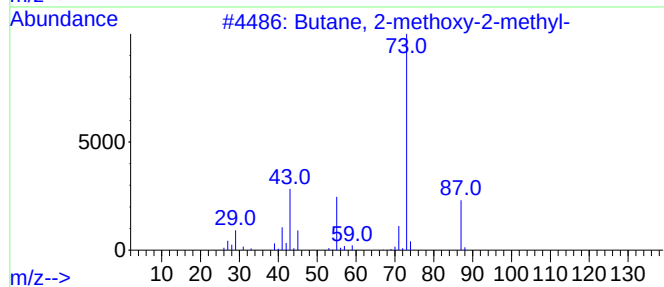
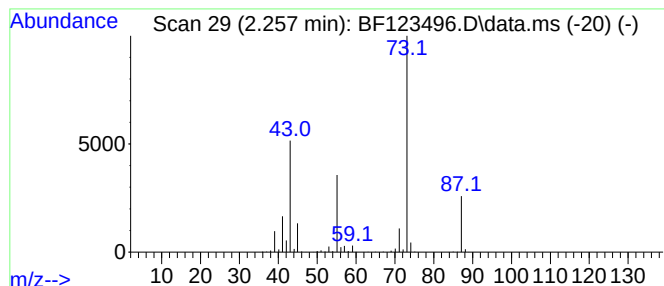
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	21.04 ng	1663490	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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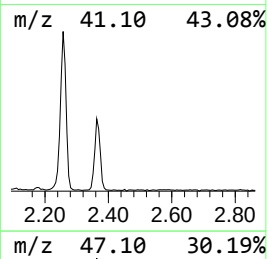
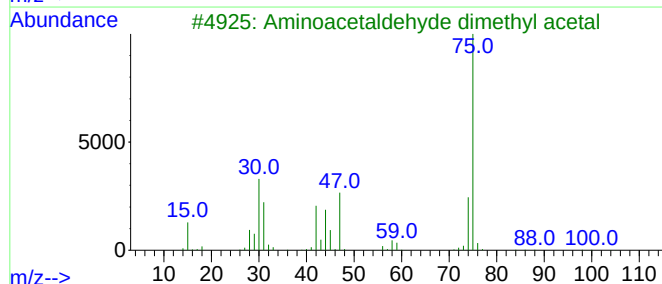
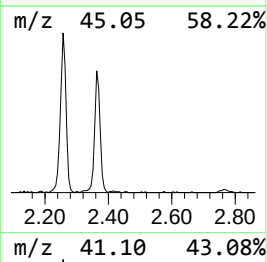
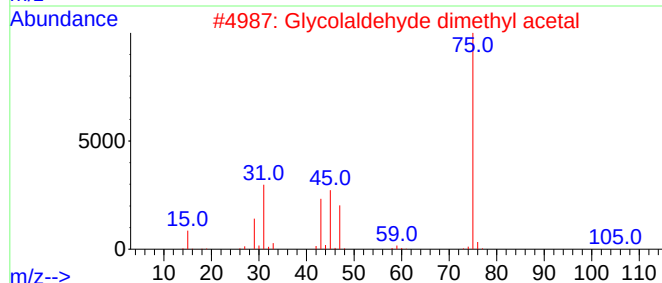
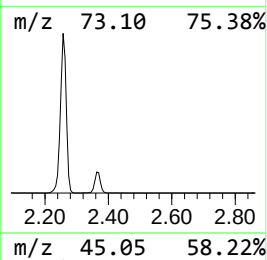
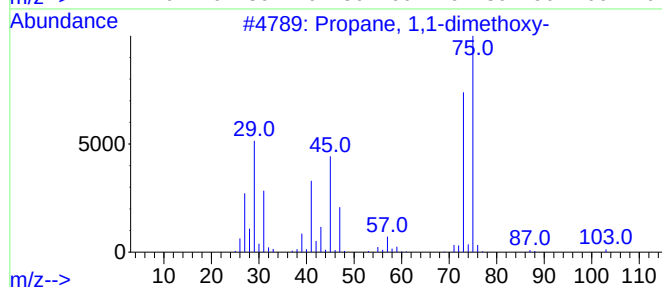
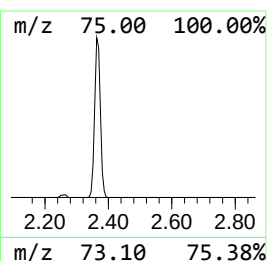
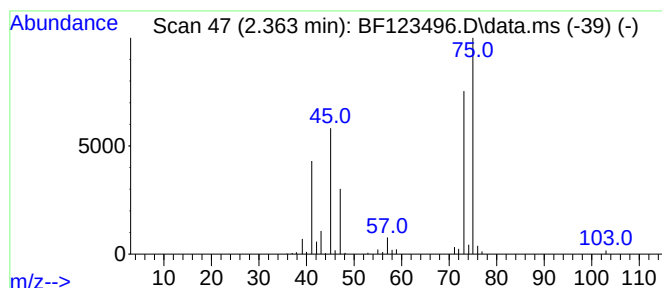
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.363	4.45 ng	351923	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	36
3	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
4	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	33
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22



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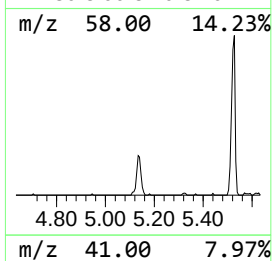
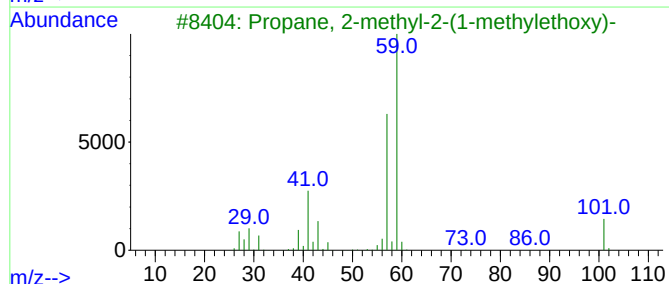
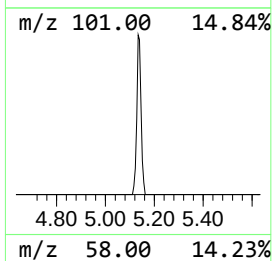
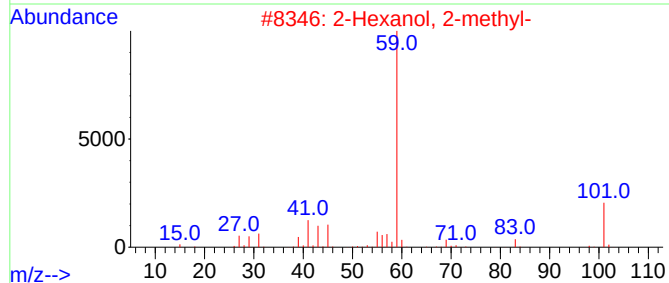
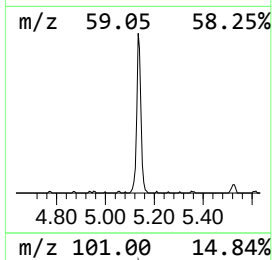
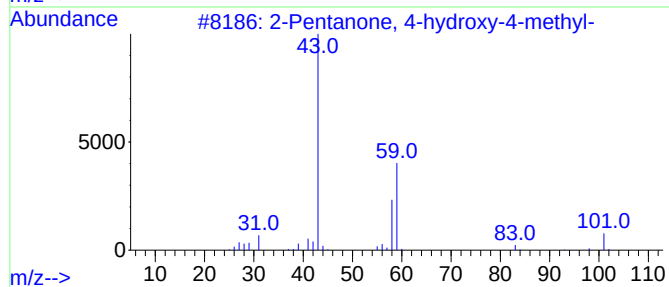
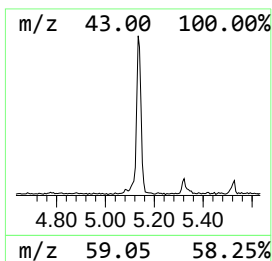
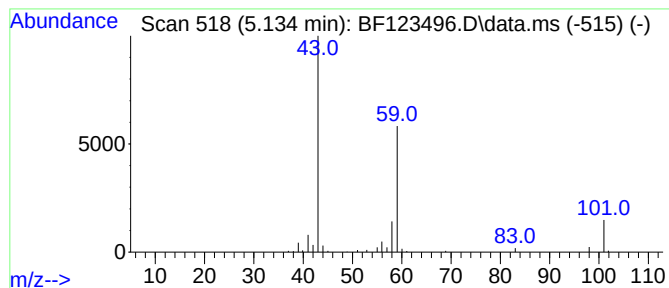
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	2.39 ng	188626	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
4	Butane	58	C4H10	000106-97-8	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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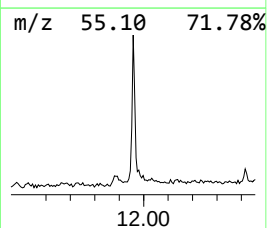
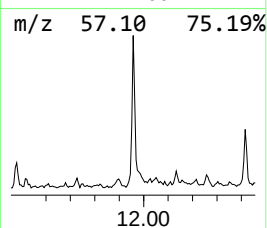
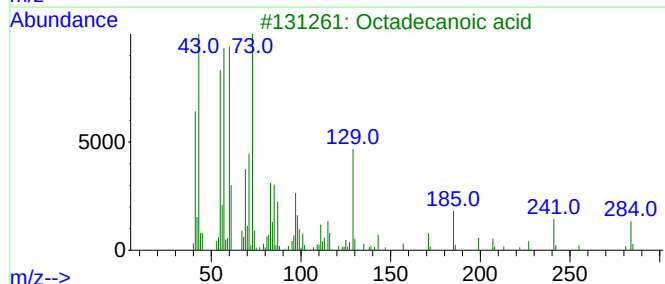
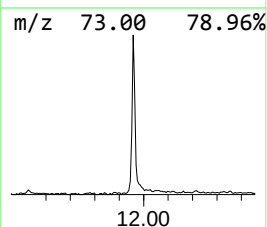
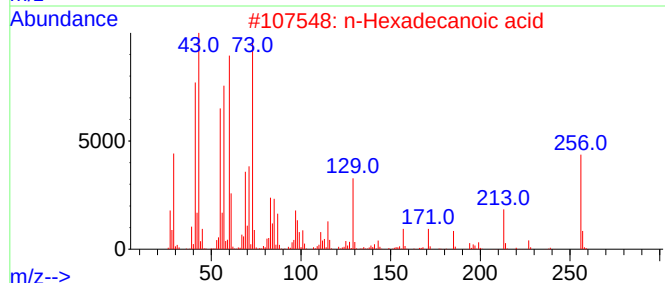
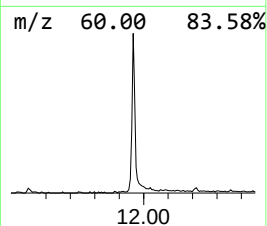
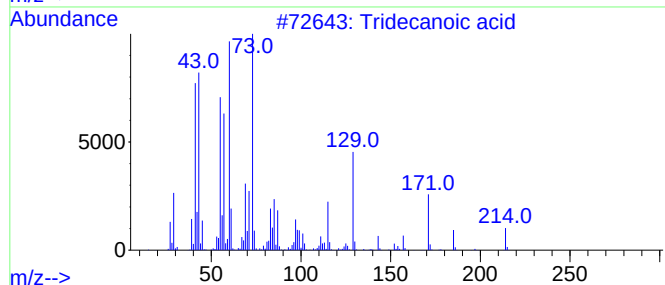
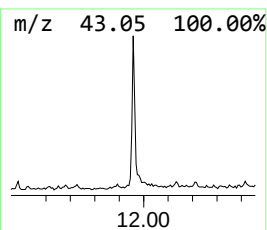
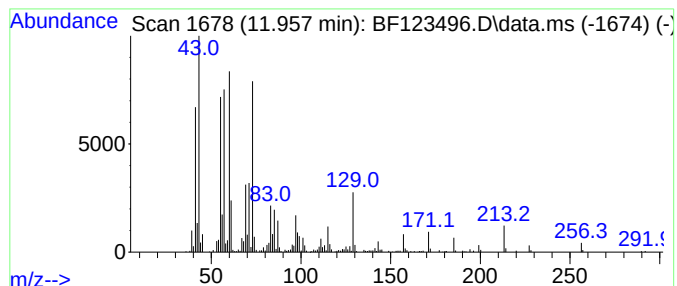
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	6.07 ng	649000	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Octadecanoic acid	284	C18H36O2	000057-11-4	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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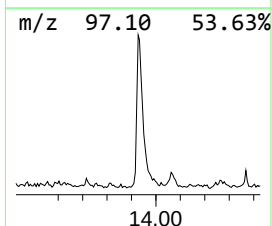
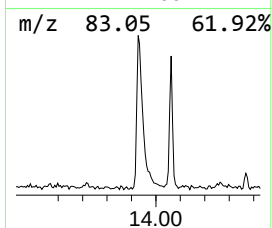
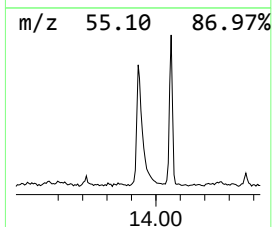
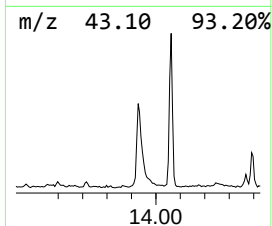
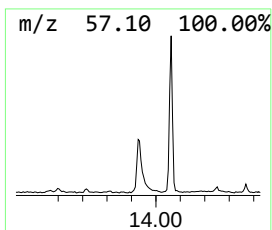
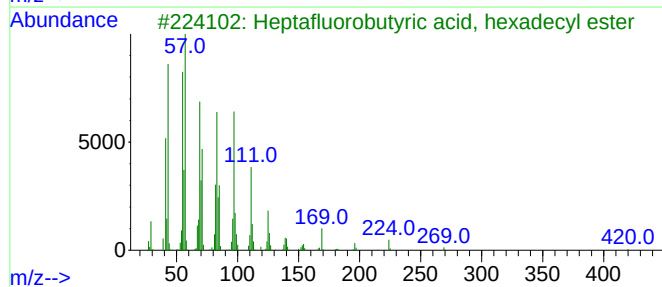
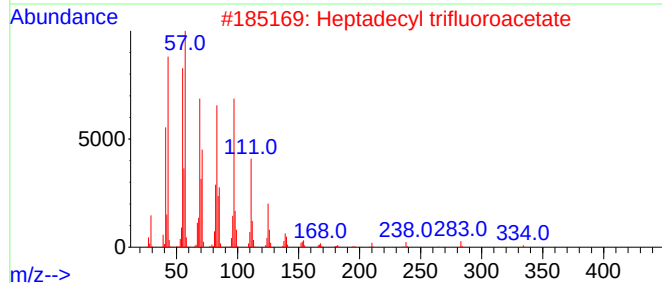
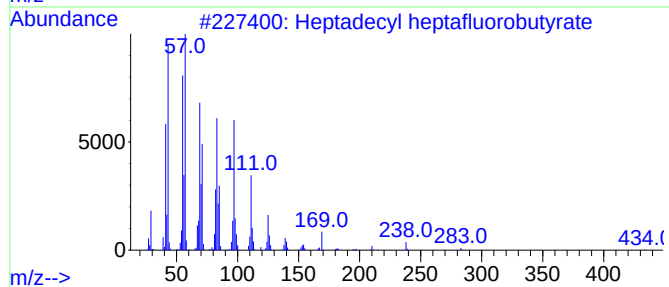
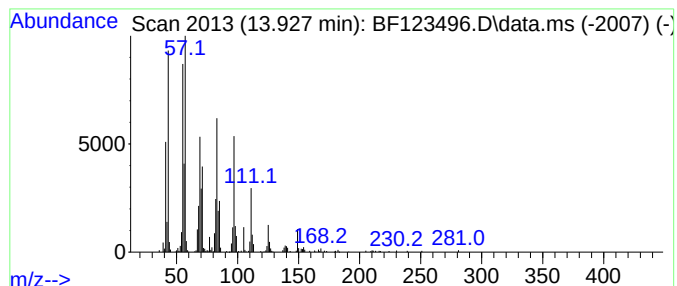
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	15.57 ng	1194050	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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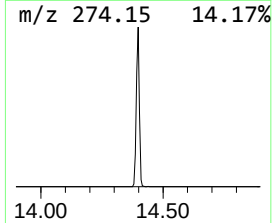
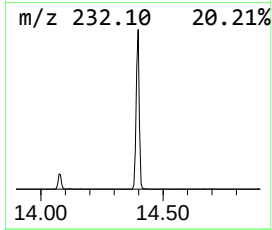
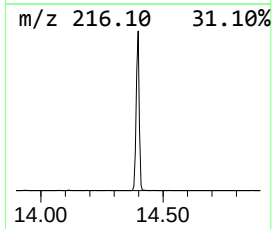
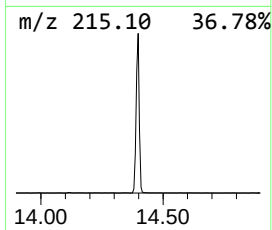
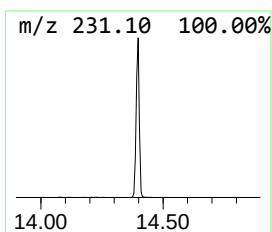
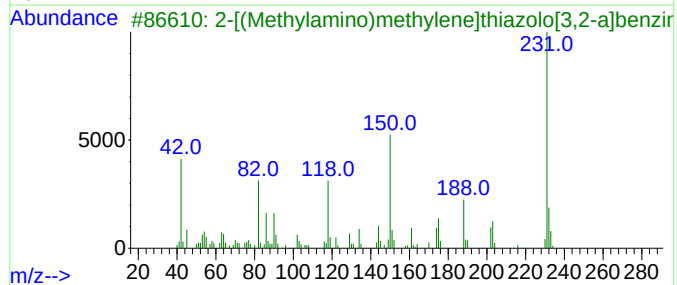
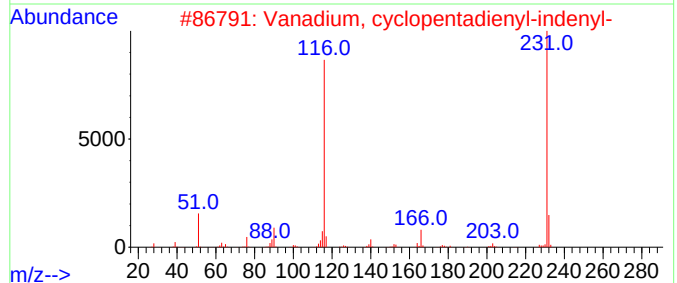
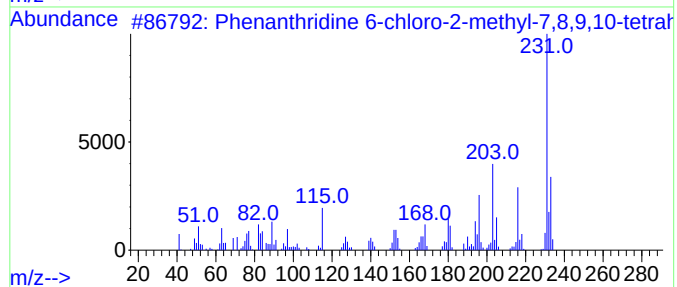
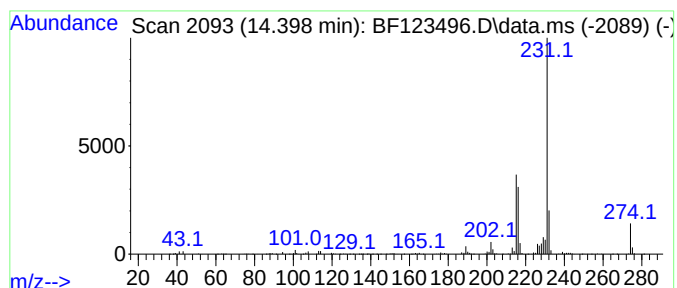
Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenanthridine 6-chloro-2-m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.398	40.18 ng	3082000	Chrysene-d12	14.074	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthridine 6-chloro-2-methyl...	231	C14H14ClN	035417-77-7	53
2	Vanadium, cyclopentadienyl-indenyl-	231	C14H12V	1000152-33-3	49
3	2-[(Methylamino)methylene]thiazo...	231	C11H9N3OS	072740-41-1	49
4	Furane-2-carboxaldehyde, 5-(2-me...	231	C12H9NO4	329222-70-0	47
5	1H-Indole-3-methanamine, 5-ethyl...	274	C16H26N2Si	074367-52-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123496.D
Acq On : 26 Mar 2021 20:35
Operator : JU/CG
Sample : M1792-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

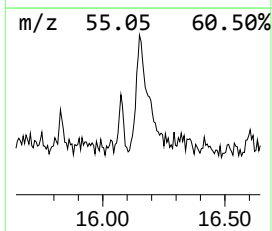
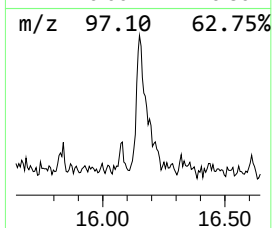
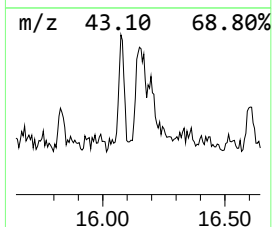
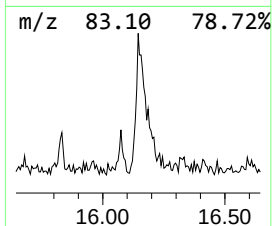
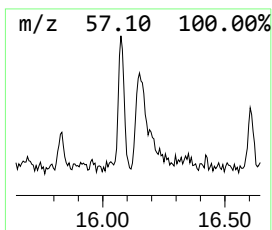
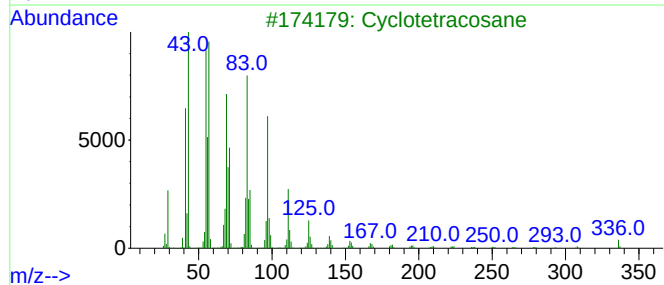
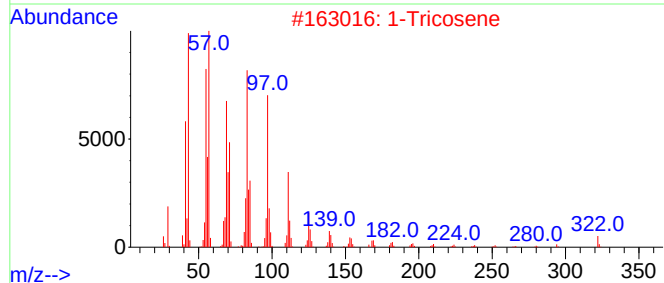
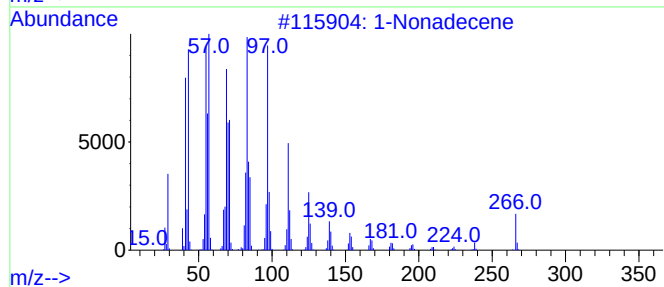
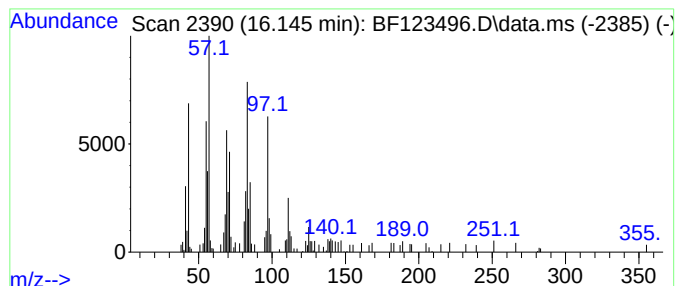
Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.145	3.79 ng	247324	Perylene-d12	15.574	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	1-Tricosene	322	C23H46	018835-32-0	90
3	Cyclotetracosane	336	C24H48	000297-03-0	87
4	17-Pentatriacontene	491	C35H70	006971-40-0	87
5	1-Hexacosanol	382	C26H54O	000506-52-5	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123496.D
Acq On : 26 Mar 2021 20:35
Operator : JU/CG
Sample : M1792-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
TP-5

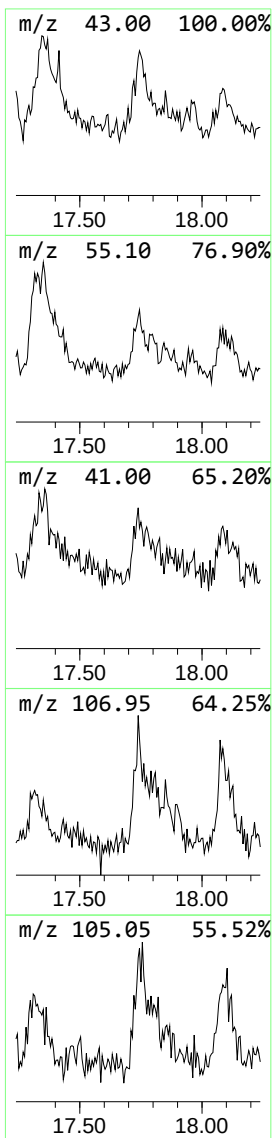
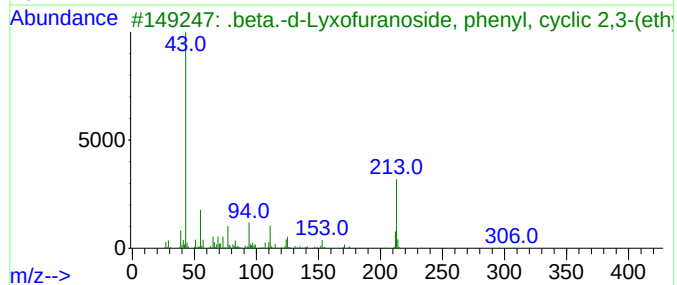
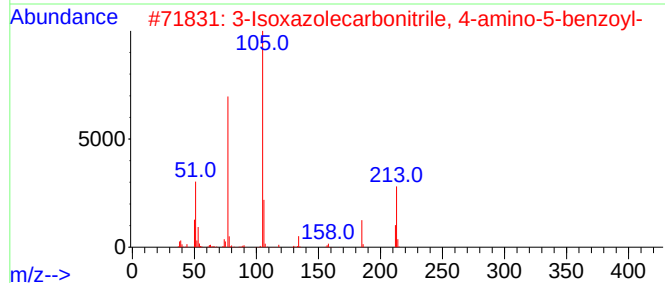
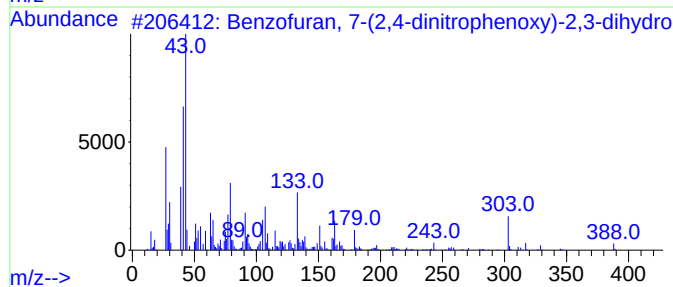
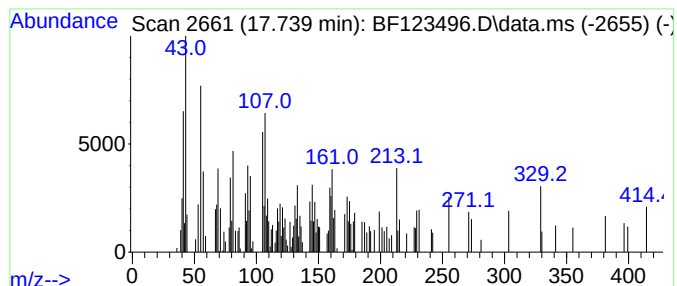
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.739 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.739	3.17 ng	206926	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzofuran, 7-(2,4-dinitrophenox...	388	C19H20N2O7	062059-48-7	10
2			3-Isoxazolecarbonitrile, 4-amino...	213	C11H7N3O2	1000351-57-9	10
3			.beta.-d-Lyxofuranoside, phenyl...	306	C15H19B06	128902-53-4	9
4			Hydroxy-(3-methoxyphenyl)phenyla...	272	C16H16O4	1000288-01-3	9
5			Benzeneethanoic acid, .alpha.-(4...	258	C15H14O4	004237-50-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123496.D
Acq On : 26 Mar 2021 20:35
Operator : JU/CG
Sample : M1792-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
TP-5

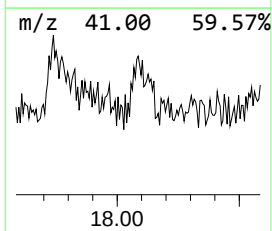
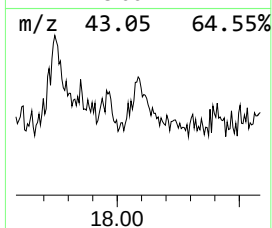
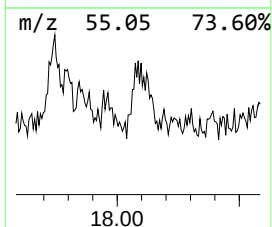
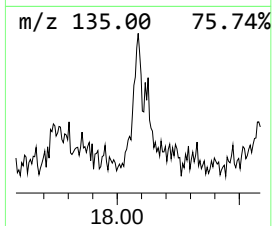
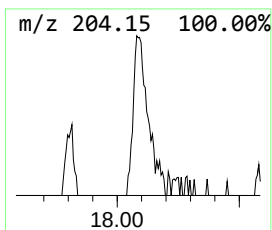
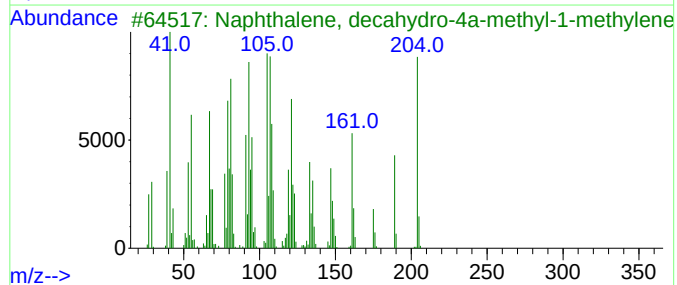
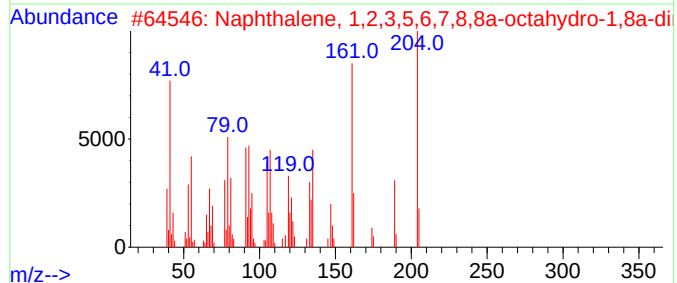
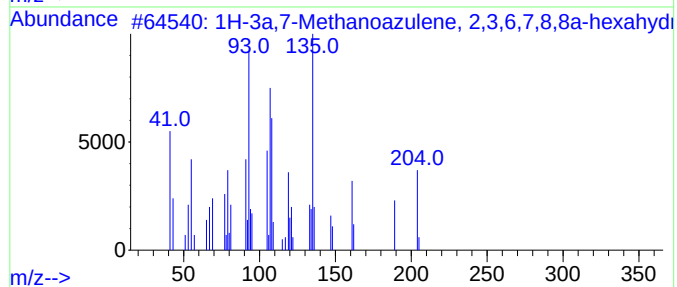
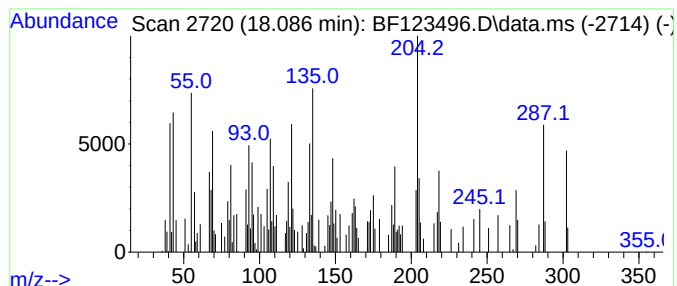
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown18.086 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.086	4.54 ng	295703	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	43
2			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	43
3			Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	41
4			Aromandendrene	204	C15H24	000489-39-4	41
5			2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H200	124957-09-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123496.D
Acq On : 26 Mar 2021 20:35
Operator : JU/CG
Sample : M1792-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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...	2.257	21.0	ng	1663490	1	6.898	1581220	20.0
Propane, 1,1-di...	2.363	4.5	ng	351923	1	6.898	1581220	20.0
2-Pentanone, 4-...	5.134	2.4	ng	188626	1	6.898	1581220	20.0
Tridecanoic acid	11.957	6.1	ng	649000	4	11.433	2139070	20.0
Heptadecyl hept...	13.927	15.6	ng	1194050	5	14.074	1534170	20.0
Phenanthridine ...	14.398	40.2	ng	3082000	5	14.074	1534170	20.0
1-Nonadecene	16.145	3.8	ng	247324	6	15.574	1304040	20.0
unknown17.739	17.739	3.2	ng	206926	6	15.574	1304040	20.0
unknown18.086	18.086	4.5	ng	295703	6	15.574	1304040	20.0