

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063021\
 Data File : BF124495.D
 Acq On : 30 Jun 2021 16:30
 Operator : JU/CG
 Sample : M2895-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-2

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-BF062321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.881	472	475	487	rBV	85483	119226	8.83%	1.671%
2	5.316	546	549	569	rBV	663788	726415	53.82%	10.178%
3	6.345	720	724	736	rBV	828623	750227	55.59%	10.512%
4	6.687	779	782	790	rBB	215421	189120	14.01%	2.650%
5	7.257	876	879	885	rBV	602724	520054	38.53%	7.287%
6	7.975	997	1001	1006	rBV	264895	243544	18.05%	3.412%
7	9.051	1180	1184	1187	rBV	1303718	1073733	79.56%	15.045%
8	9.451	1248	1252	1260	rBB	162101	143329	10.62%	2.008%
9	9.722	1295	1298	1307	rBB	355813	314952	23.34%	4.413%
10	10.516	1430	1433	1441	rBV	752337	644576	47.76%	9.032%
11	11.210	1548	1551	1555	rBV	395843	344904	25.56%	4.833%
12	11.745	1638	1642	1645	rBV2	40723	40763	3.02%	0.571%
13	12.180	1712	1716	1719	rBV	17432	17386	1.29%	0.244%
14	12.798	1816	1821	1824	rBV	1493666	1349616	100.00%	18.910%
15	13.704	1969	1975	1976	rBV3	41308	45693	3.39%	0.640%
16	13.727	1977	1979	1990	rVB5	42498	81718	6.05%	1.145%
17	13.857	1998	2001	2008	rVB	367295	314821	23.33%	4.411%
18	15.286	2240	2244	2254	rBV	179065	216813	16.06%	3.038%

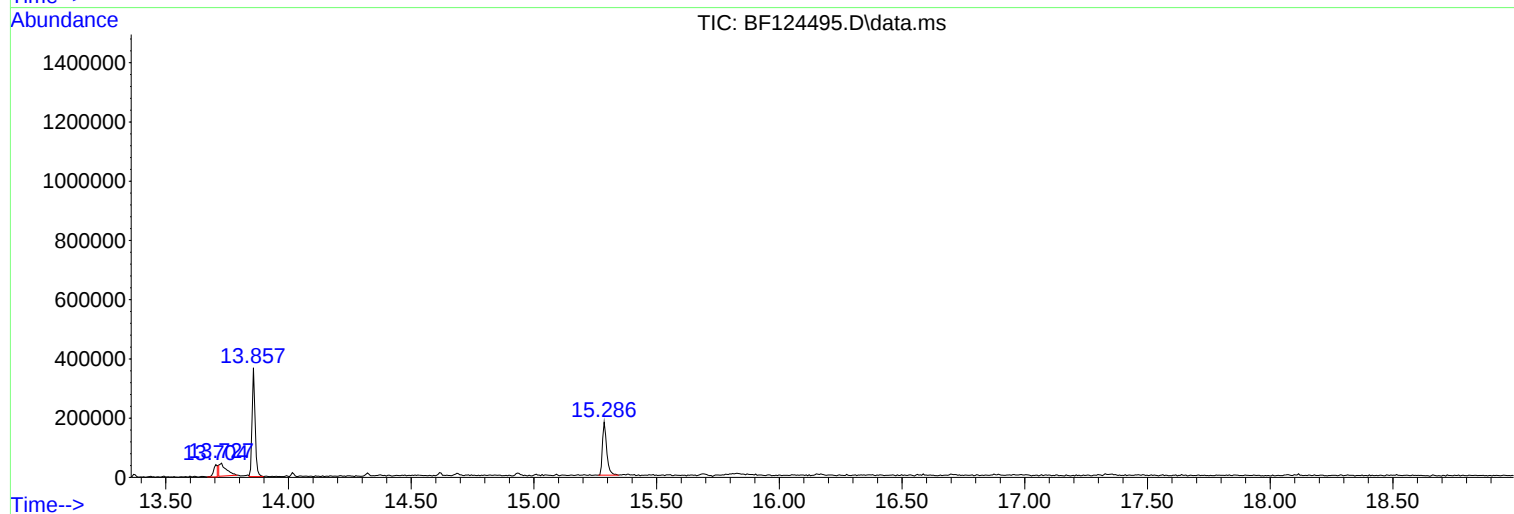
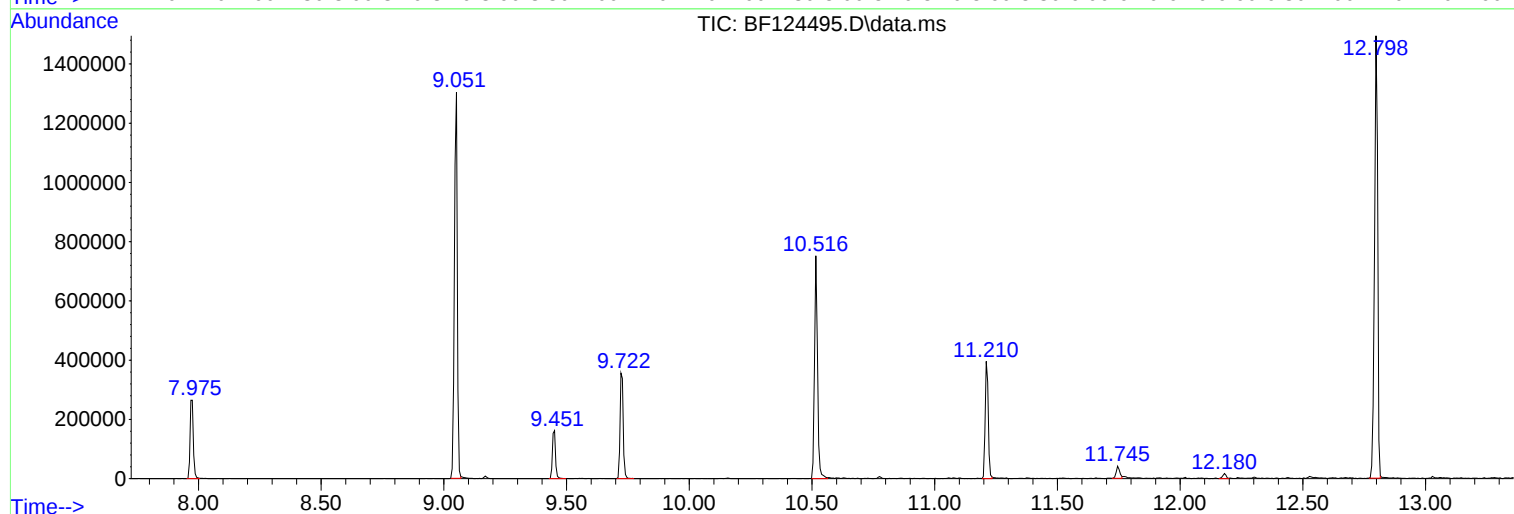
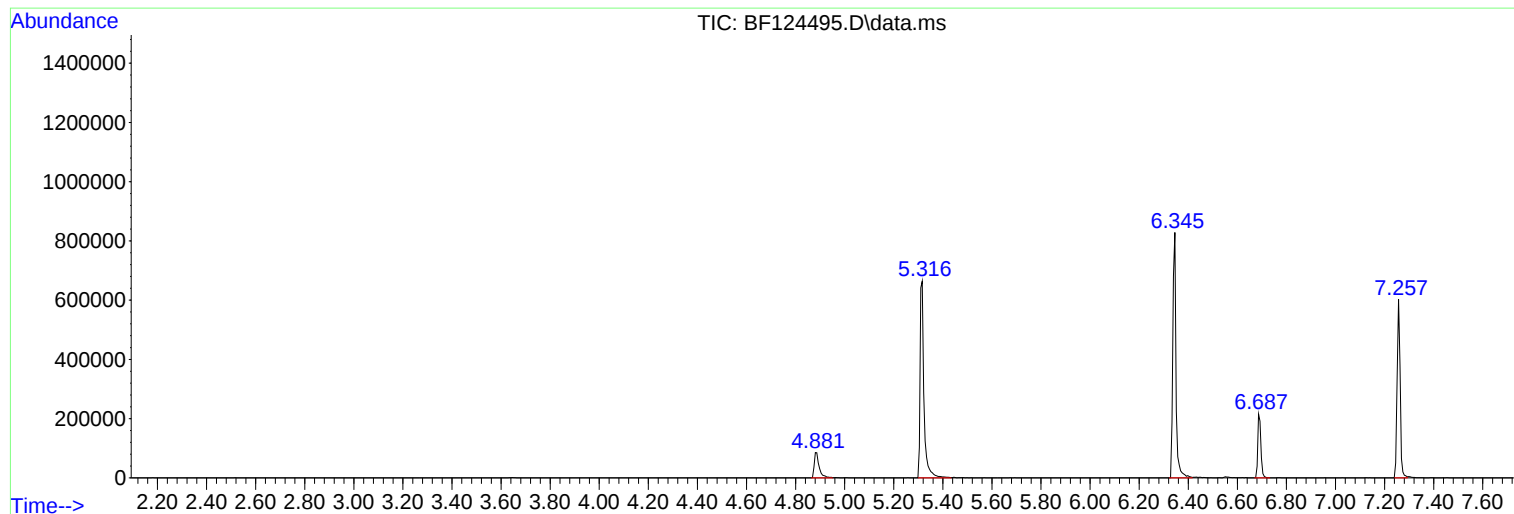
Sum of corrected areas: 7136890

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063021\
Data File : BF124495.D
Acq On : 30 Jun 2021 16:30
Operator : JU/CG
Sample : M2895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063021\
Data File : BF124495.D
Acq On : 30 Jun 2021 16:30
Operator : JU/CG
Sample : M2895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

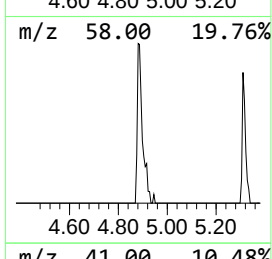
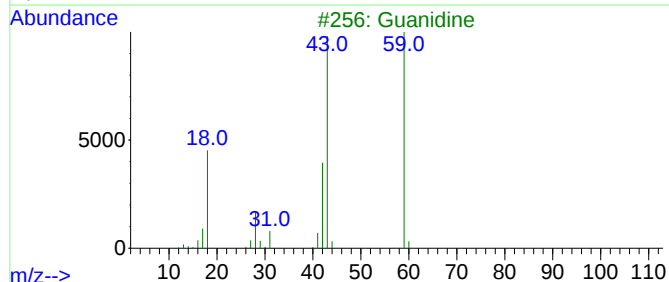
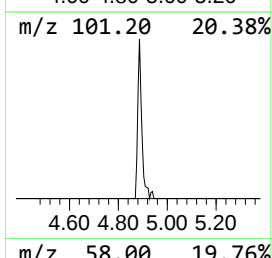
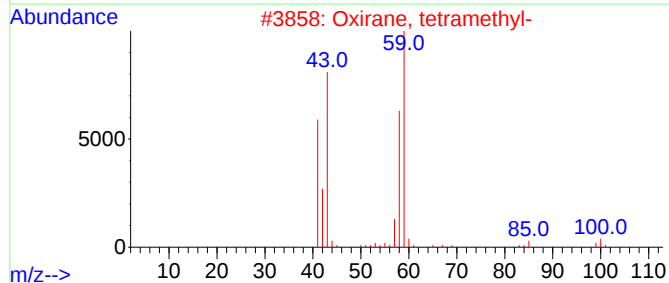
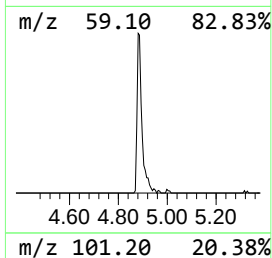
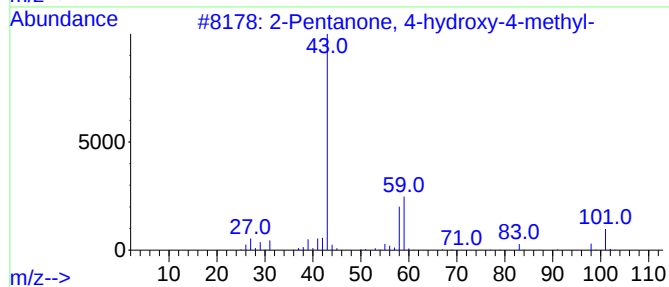
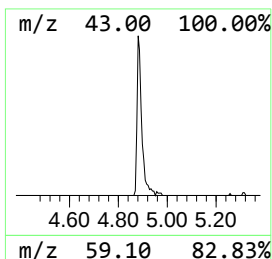
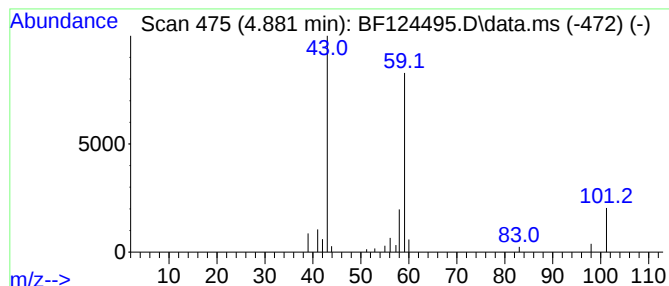
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.881	12.61 ng	119226	1,4-Dichlorobenzene-d4	6.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	28		
3	Guanidine	59	CH5N3	000113-00-8	9		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9		
5	3-Octanol	130	C8H18O	000589-98-0	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063021\
Data File : BF124495.D
Acq On : 30 Jun 2021 16:30
Operator : JU/CG
Sample : M2895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

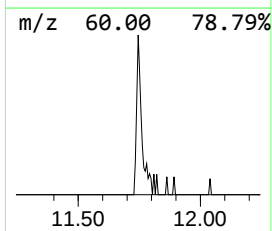
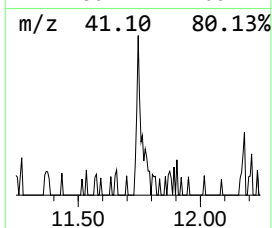
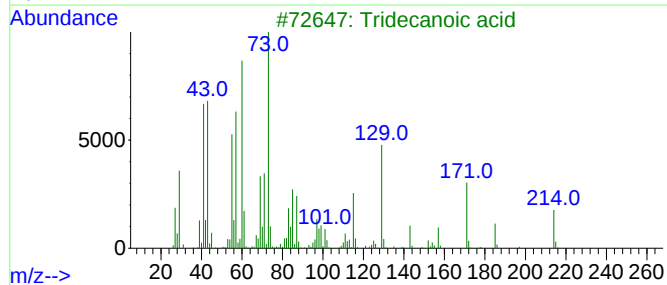
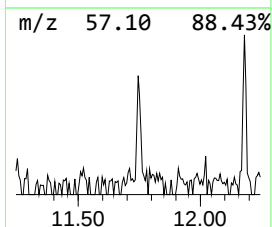
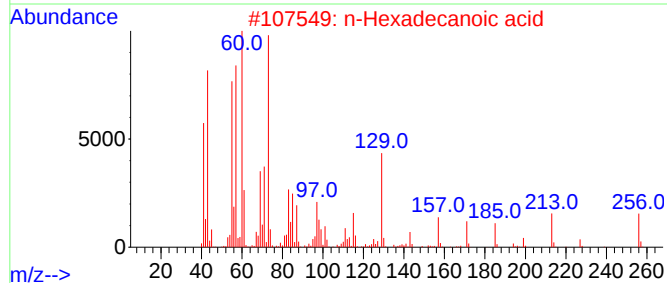
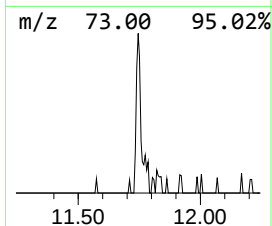
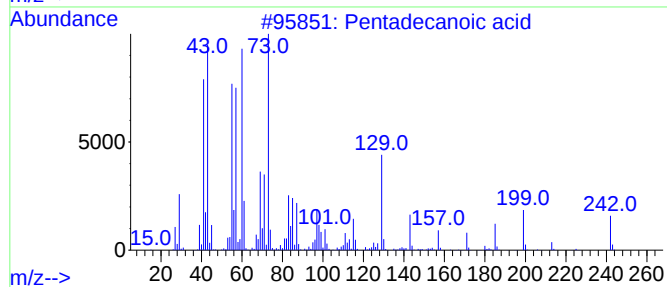
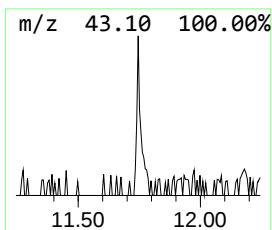
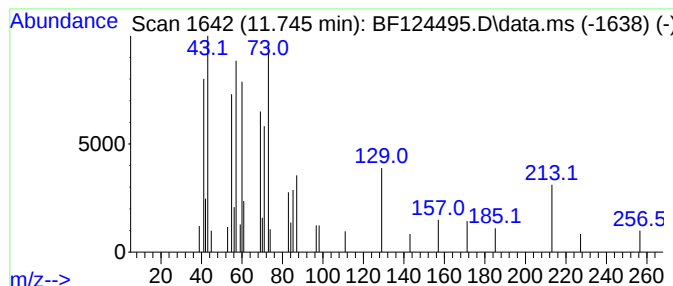
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.745	2.36 ng	40763	Phenanthrene-d10	11.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Dodecanoic acid	200	C12H24O2	000143-07-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063021\
Data File : BF124495.D
Acq On : 30 Jun 2021 16:30
Operator : JU/CG
Sample : M2895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

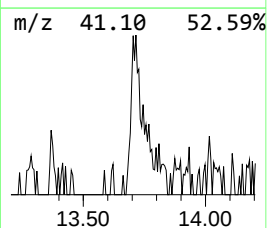
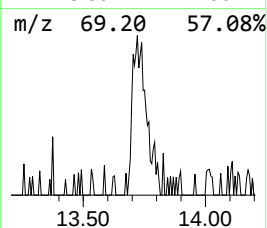
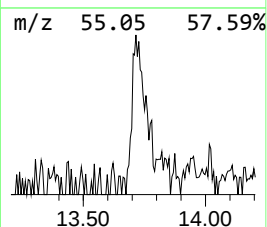
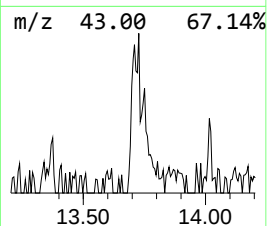
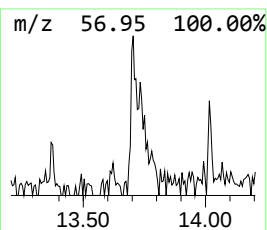
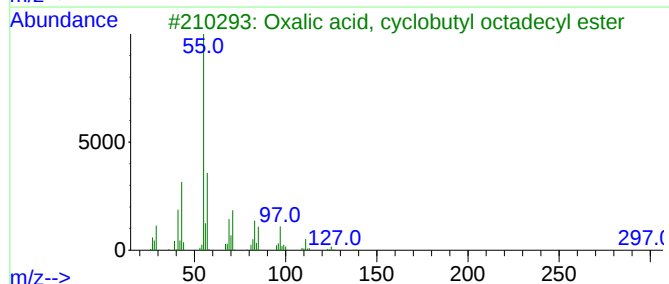
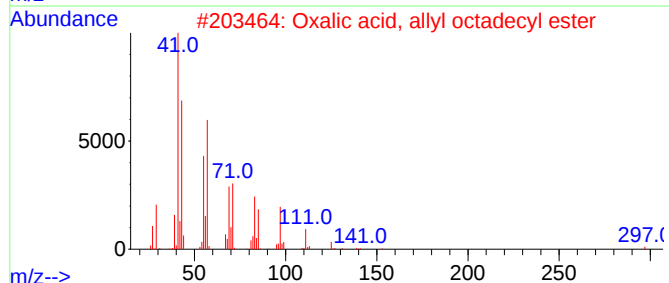
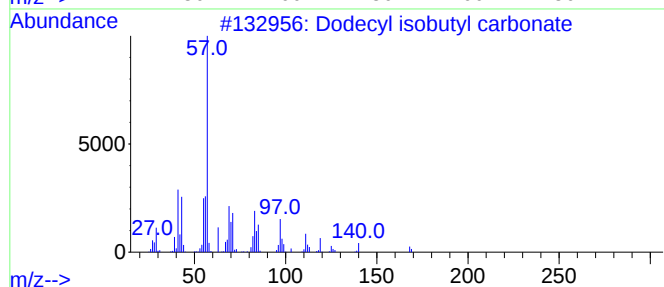
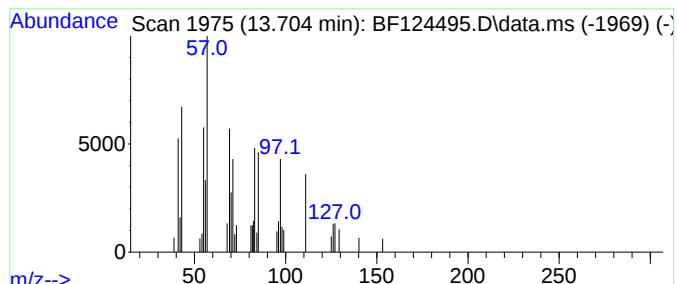
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Dodecyl isobutyl carbonate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.704	2.90 ng	45693	Chrysene-d12	13.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	72
2			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	72
3			Oxalic acid, cyclobutyl octadecyl...	396	C24H44O4	1000309-70-8	59
4			17-Pentatriacontene	491	C35H70	006971-40-0	58
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063021\
Data File : BF124495.D
Acq On : 30 Jun 2021 16:30
Operator : JU/CG
Sample : M2895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

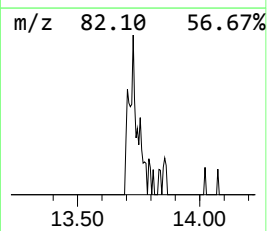
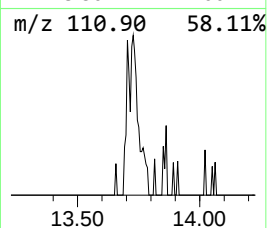
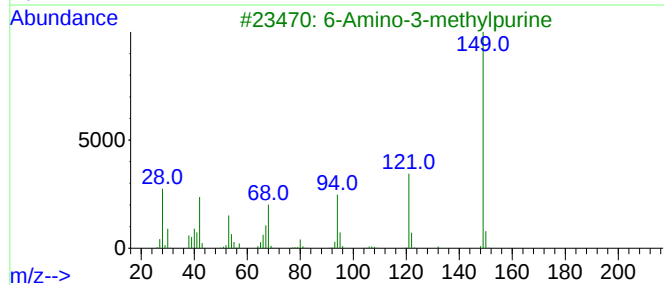
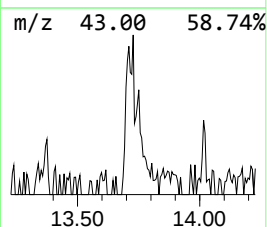
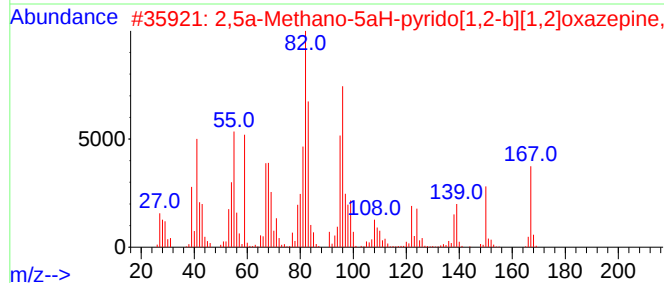
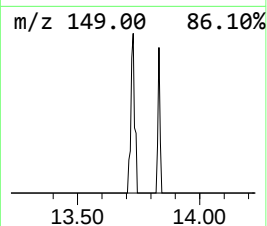
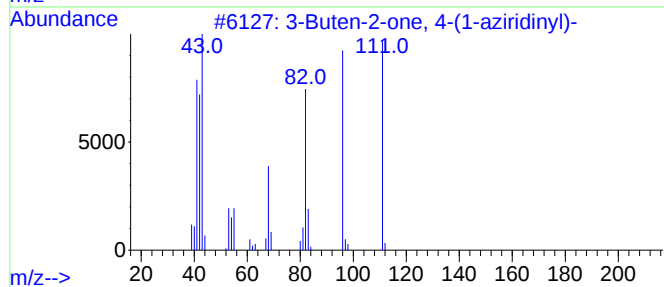
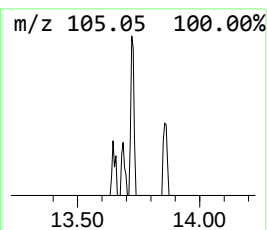
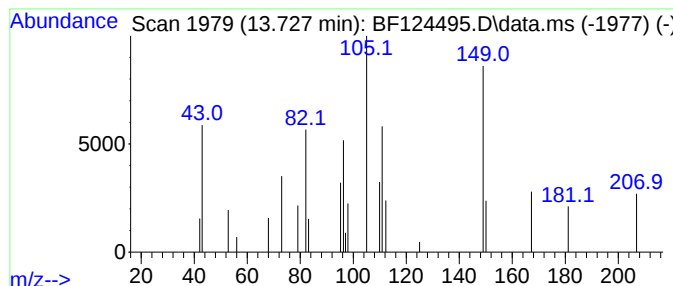
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown13.727 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	5.19 ng	81718	Chrysene-d12	13.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-one, 4-(1-aziridiny)-	111	C6H9NO	018277-57-1	10
2			2,5a-Methano-5aH-pyrido[1,2-b][1...	167	C10H17NO	054980-46-0	10
3			6-Amino-3-methylpurine	149	C6H7N5	005142-23-4	9
4			6-Fluoro-3-hydroxy-1,3-dihydro-i...	167	C8H6FN02	1000274-99-6	9
5			2-Fluoro-3-methylpyridine	111	C6H6FN	017282-04-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063021\
Data File : BF124495.D
Acq On : 30 Jun 2021 16:30
Operator : JU/CG
Sample : M2895-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062321.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
2-Pentanone, 4-...	4.881	12.6	ng	119226	1	6.692	189120	20.0
Pentadecanoic acid	11.745	2.4	ng	40763	4	11.210	344904	20.0
Dodecyl isobuty...	13.704	2.9	ng	45693	5	13.857	314821	20.0
unknown13.727	13.727	5.2	ng	81718	5	13.857	314821	20.0