

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
 Data File : BF136453.D
 Acq On : 07 Dec 2023 18:29
 Operator : CG\JU
 Sample : 05599-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LKWD-BACKFILL-03

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-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136453.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	18	21	28	rVB	32729	43336	1.66%	0.274%
2	5.040	498	502	509	rVB	186991	201607	7.73%	1.276%
3	5.445	566	571	574	rBV	2173336	1974061	75.73%	12.492%
4	6.445	736	741	744	rBV	2190033	1991876	76.41%	12.605%
5	6.798	798	801	804	rBV	840624	652543	25.03%	4.129%
6	7.363	891	897	900	rBV	1344849	1347326	51.69%	8.526%
7	8.075	1014	1018	1022	rBV	1041197	841128	32.27%	5.323%
8	8.392	1068	1072	1080	rBV2	21705	36534	1.40%	0.231%
9	9.157	1197	1202	1205	rBV	3007612	2606747	100.00%	16.496%
10	9.833	1313	1317	1320	rBV	1017152	817558	31.36%	5.174%
11	10.622	1447	1451	1464	rBV	1162778	1047503	40.18%	6.629%
12	11.321	1567	1570	1574	rBV	804840	682462	26.18%	4.319%
13	12.921	1837	1842	1845	rBV	2536160	2077374	79.69%	13.146%
14	13.862	1998	2002	2010	rBV4	53928	113798	4.37%	0.720%
15	13.974	2017	2021	2025	rBV	701300	647285	24.83%	4.096%
16	14.074	2034	2038	2045	rVB	69579	81587	3.13%	0.516%
17	14.451	2100	2102	2107	rBV5	37064	43644	1.67%	0.276%
18	14.845	2166	2169	2173	rBV2	49378	55374	2.12%	0.350%
19	15.456	2269	2273	2278	rBV	424666	540478	20.73%	3.420%

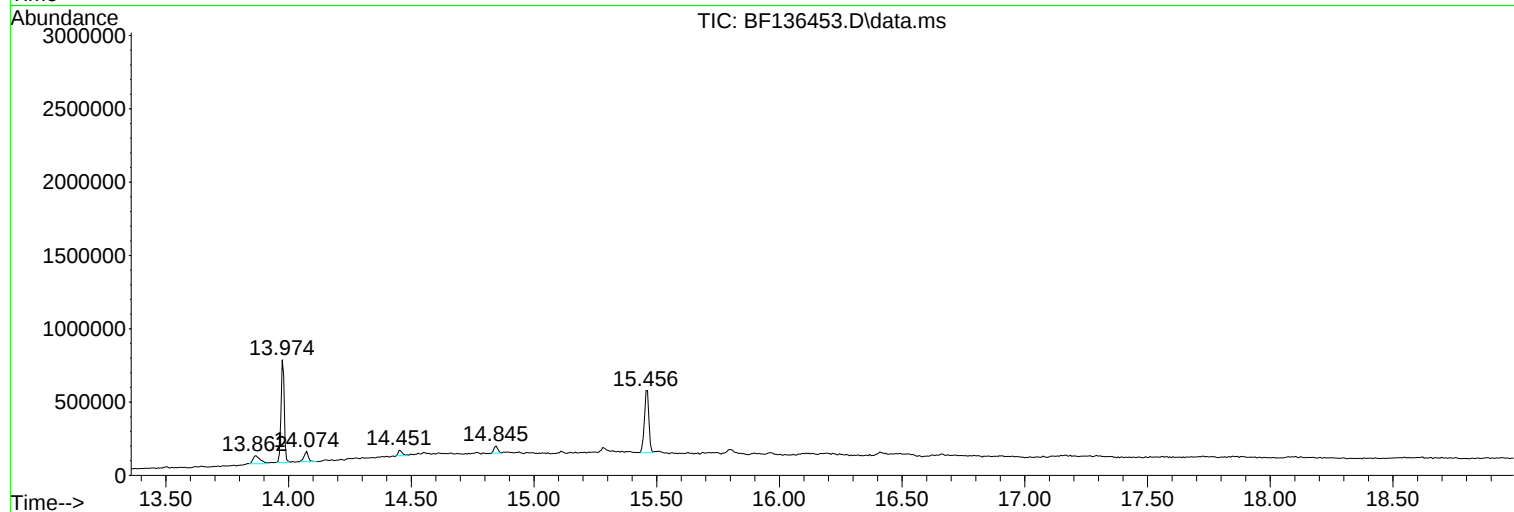
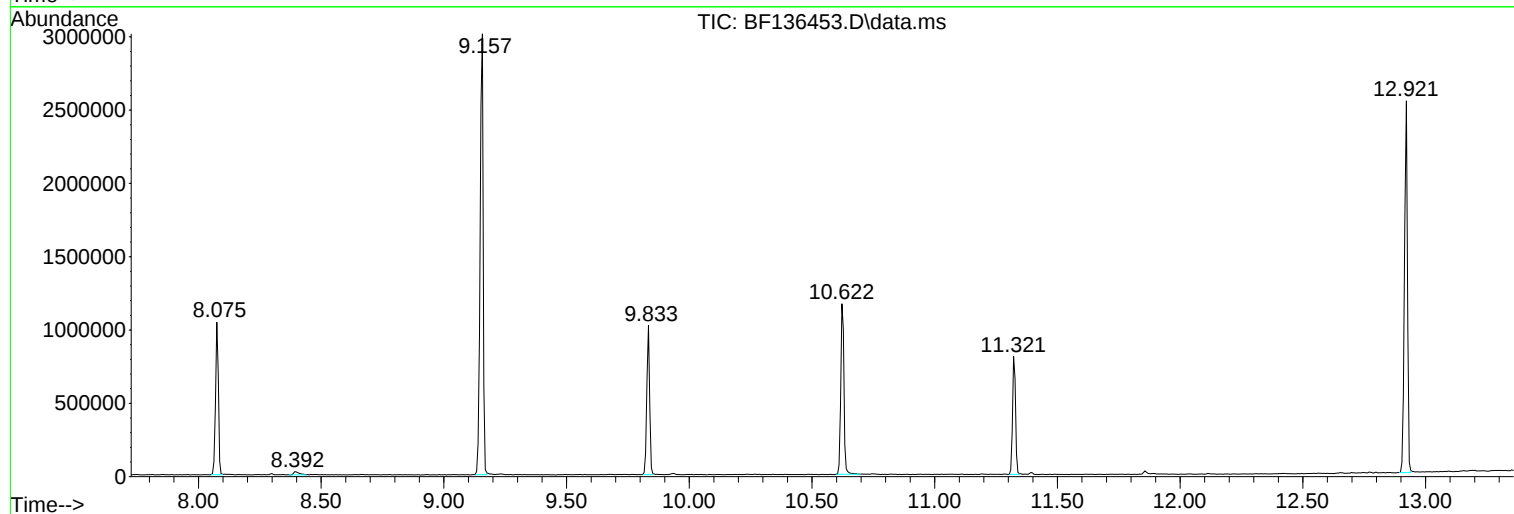
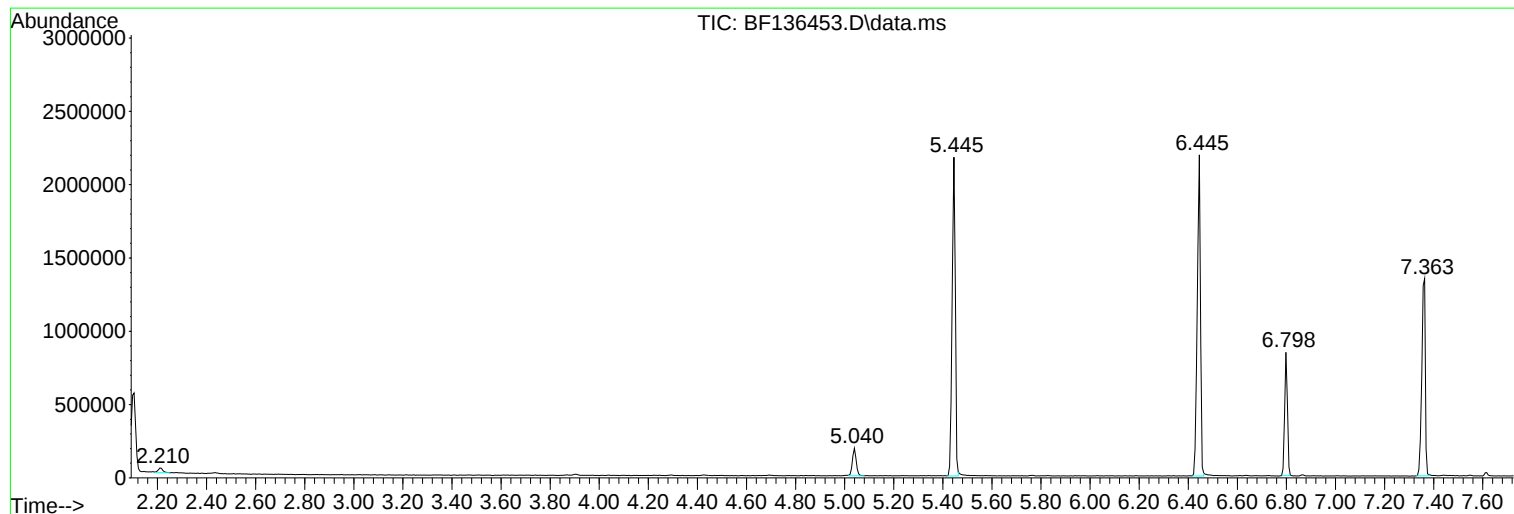
Sum of corrected areas: 15802221

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136453.D
Acq On : 07 Dec 2023 18:29
Operator : CG\JU
Sample : 05599-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136453.D
Acq On : 07 Dec 2023 18:29
Operator : CG\JU
Sample : 05599-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-03

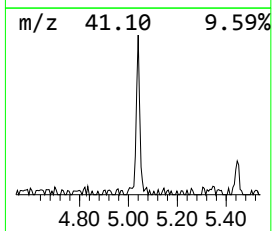
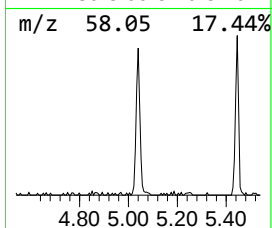
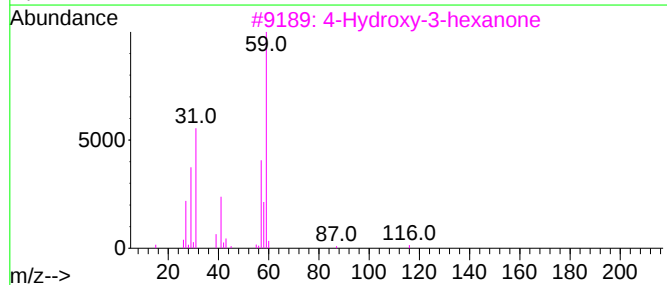
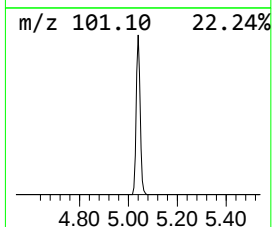
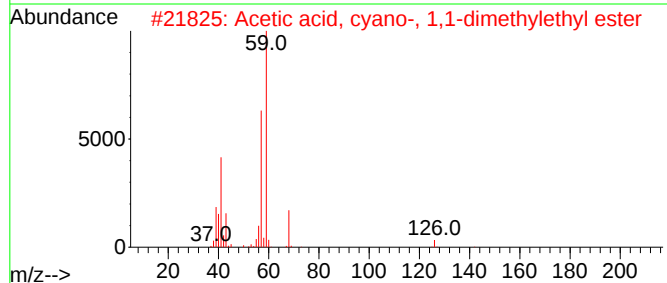
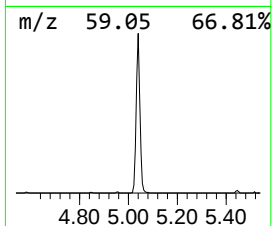
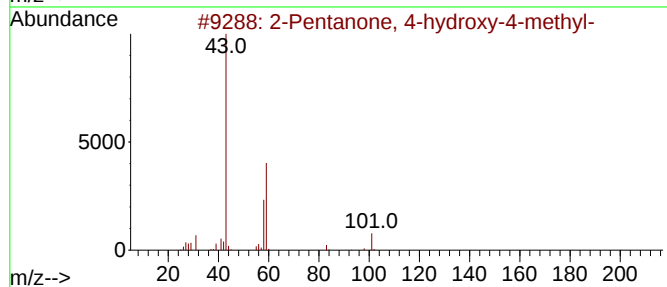
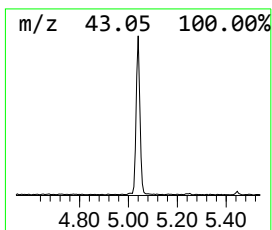
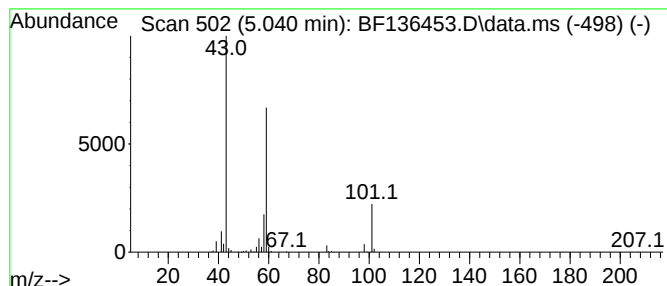
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
5.040	6.18 ng	201607	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23		
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17		
5	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	17		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136453.D
Acq On : 07 Dec 2023 18:29
Operator : CG\JU
Sample : 05599-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-03

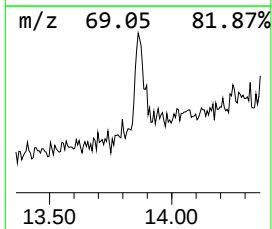
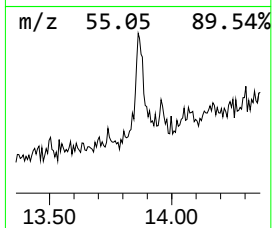
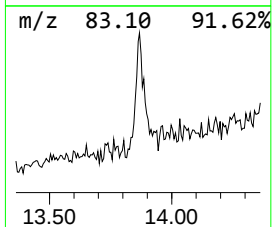
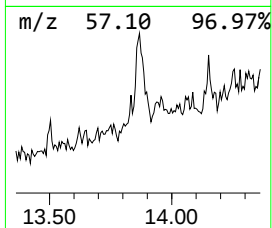
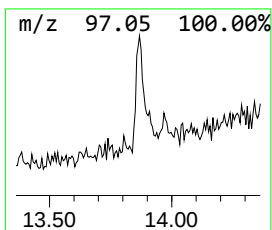
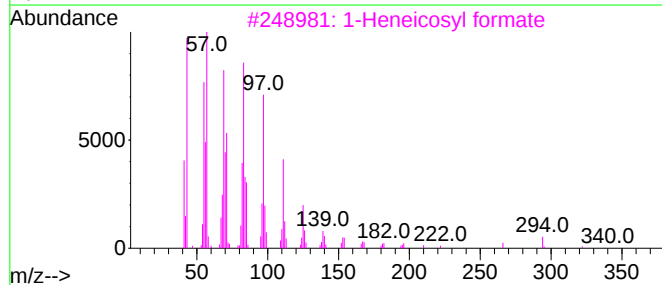
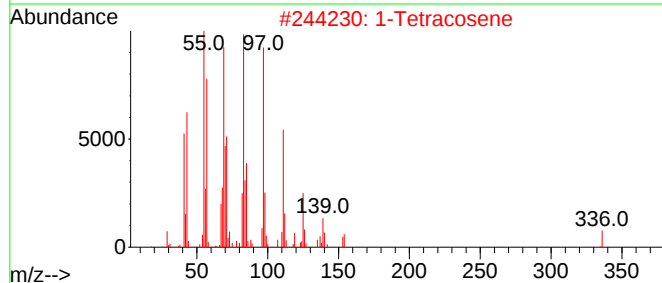
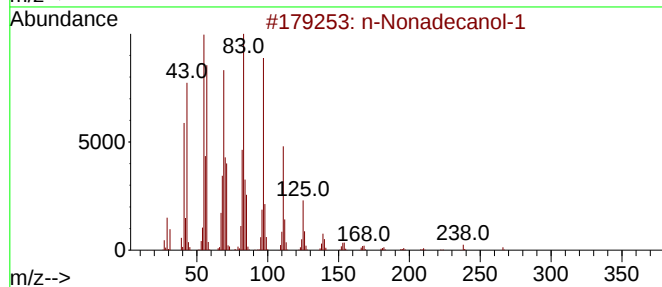
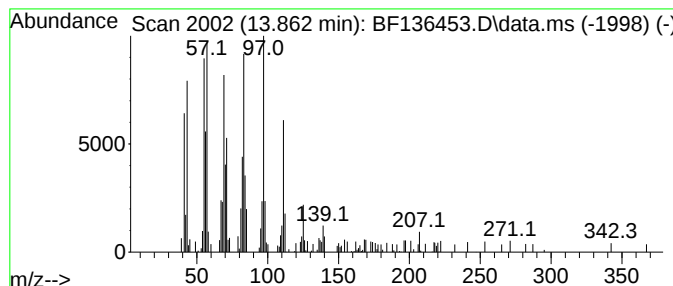
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Nonadecanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	3.52 ng	113798	Chrysene-d12	13.974

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2		1-Tetracosene	336	C24H48	010192-32-2	91
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4		Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1010164-49-7	91
5		Cyclohexadecane	224	C16H32	000295-65-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136453.D
Acq On : 07 Dec 2023 18:29
Operator : CG\JU
Sample : 05599-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-03

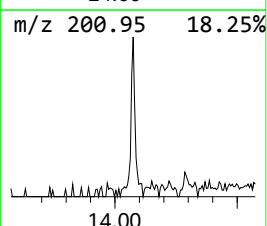
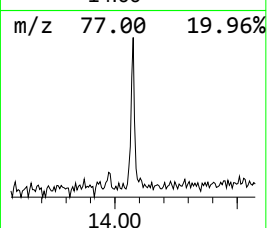
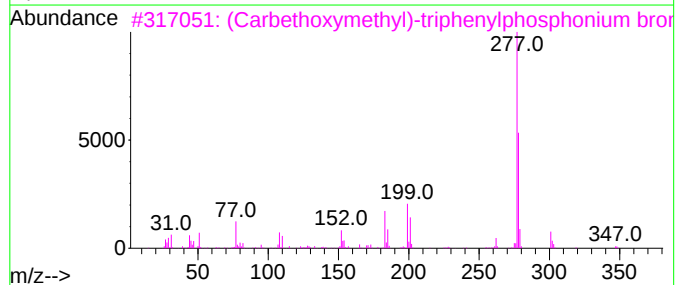
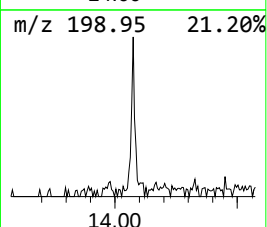
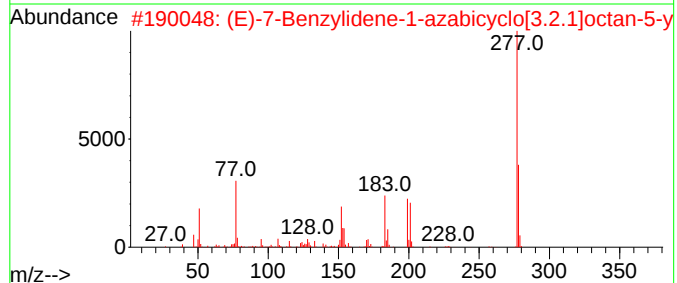
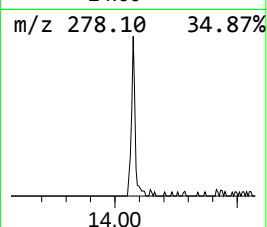
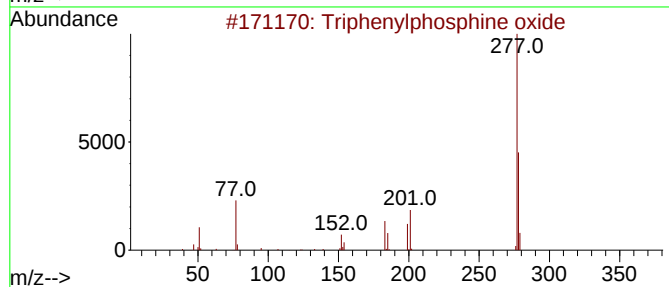
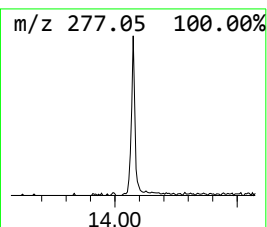
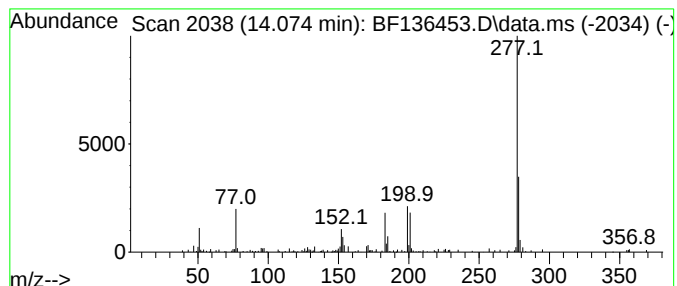
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	2.52 ng	81587	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	42
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	40
5			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136453.D
Acq On : 07 Dec 2023 18:29
Operator : CG\JU
Sample : 05599-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-03

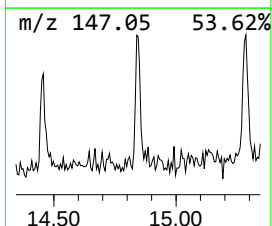
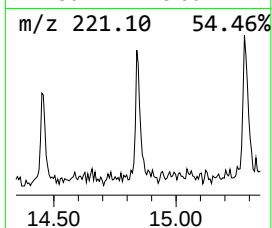
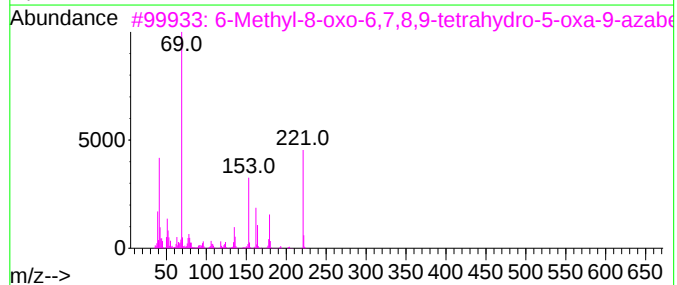
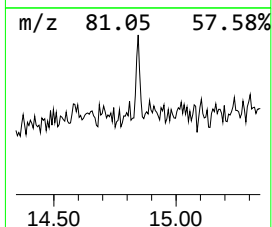
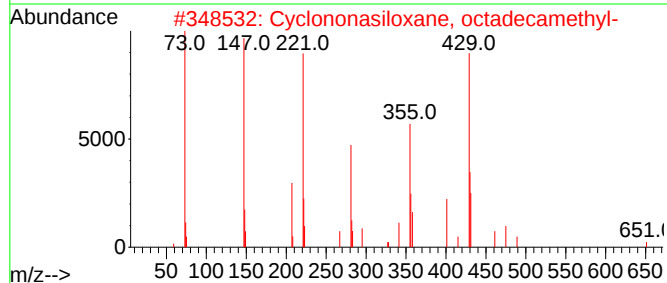
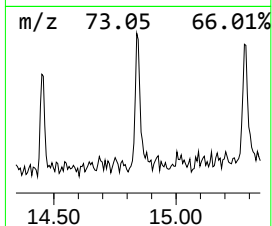
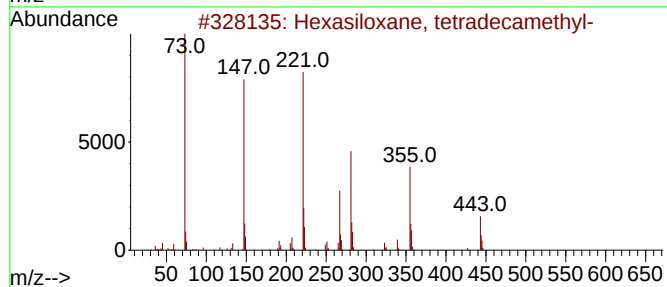
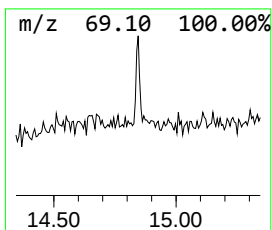
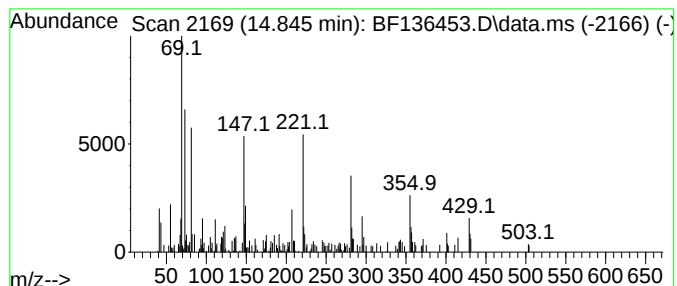
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown14.845 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	2.05 ng	55374	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	45
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38
3			6-Methyl-8-oxo-6,7,8,9-tetrahydr...	221	C11H11NO4	134076-69-0	32
4			ethanol, 2-[(6-nitro-1,3-benzod...	238	C10H10N2O5	1000396-45-9	22
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136453.D
Acq On : 07 Dec 2023 18:29
Operator : CG\JU
Sample : 05599-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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
2-Pentanone, 4-...	5.040	6.2	ng	201607	1	6.798	652543	20.0
n-Nonadecanol-1	13.863	3.5	ng	113798	5	13.974	647285	20.0
Triphenylphosph...	14.074	2.5	ng	81587	5	13.974	647285	20.0
unknown14.845	14.845	2.0	ng	55374	6	15.462	540478	20.0