

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051523\
 Data File : BF133387.D
 Acq On : 15 May 2023 17:17
 Operator : CG\JU
 Sample : 02781-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MGP-WASTE-WASTER-5/12/23

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133387.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.240	361	366	373	rBV	216501	275249	1.59%	0.647%
2	4.952	472	487	489	rBV	5929498	17339712	100.00%	40.735%
3	5.328	548	551	561	rVB	1323562	1201661	6.93%	2.823%
4	6.357	722	726	737	rBV	602082	617485	3.56%	1.451%
5	6.716	784	787	793	rBV	1358359	1051283	6.06%	2.470%
6	7.287	879	884	887	rBV	2964516	2954460	17.04%	6.941%
7	7.998	1002	1005	1009	rBV	1629125	1407454	8.12%	3.306%
8	9.081	1184	1189	1192	rBV	6067777	5084880	29.33%	11.946%
9	9.751	1300	1303	1307	rBV	1939204	1557801	8.98%	3.660%
10	10.463	1421	1424	1433	rVB	928159	704156	4.06%	1.654%
11	10.539	1434	1437	1446	rBV	922108	819379	4.73%	1.925%
12	10.769	1473	1476	1483	rVB	177977	177173	1.02%	0.416%
13	11.233	1552	1555	1559	rBV	1703661	1497844	8.64%	3.519%
14	12.575	1779	1783	1793	rBV	740124	772620	4.46%	1.815%
15	12.822	1821	1825	1829	rBV	4558829	4603215	26.55%	10.814%
16	13.874	1999	2004	2012	rVV	1089515	1108207	6.39%	2.603%
17	14.716	2144	2147	2153	rBV	275772	295453	1.70%	0.694%
18	15.292	2240	2245	2250	rBV	898932	1099061	6.34%	2.582%

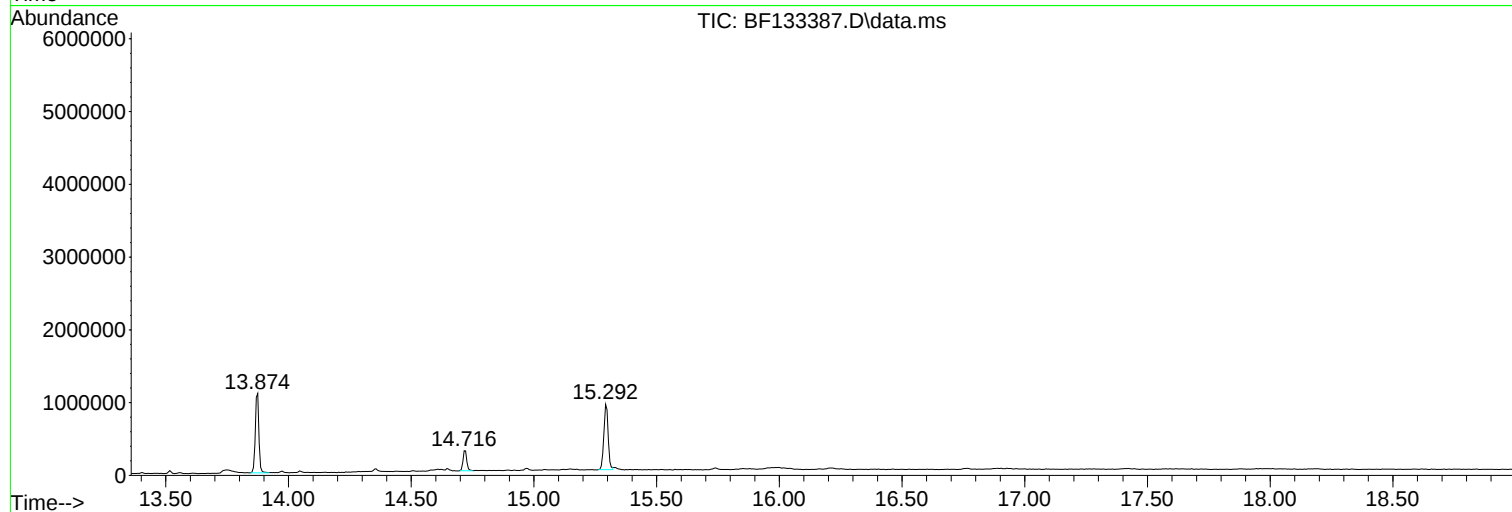
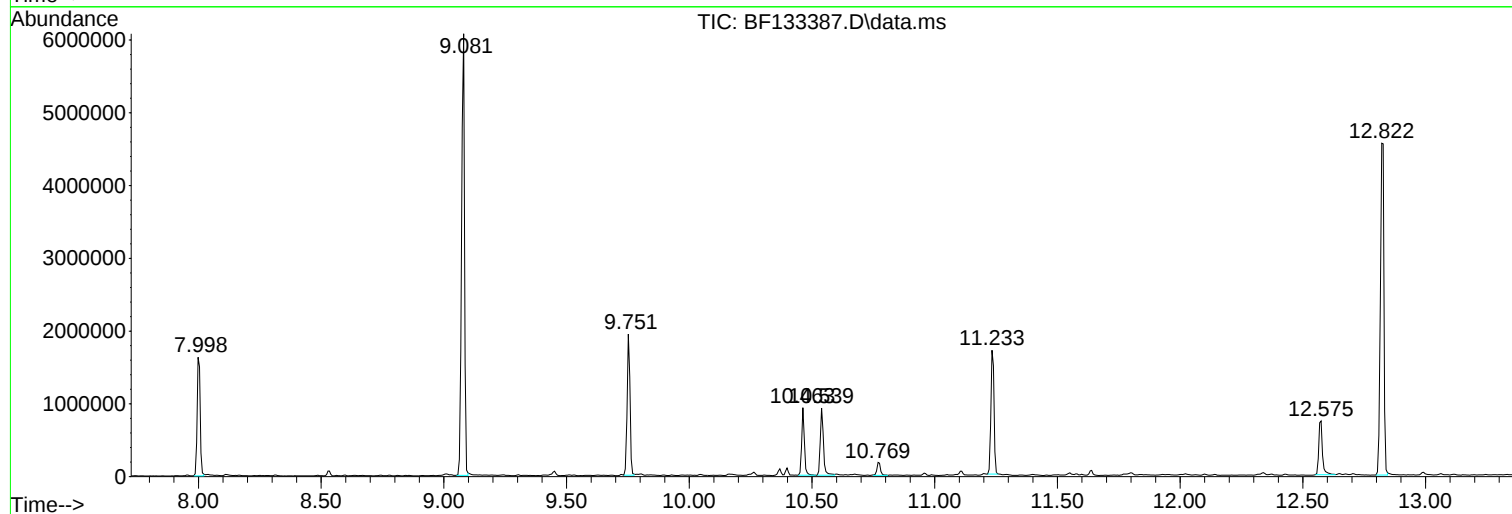
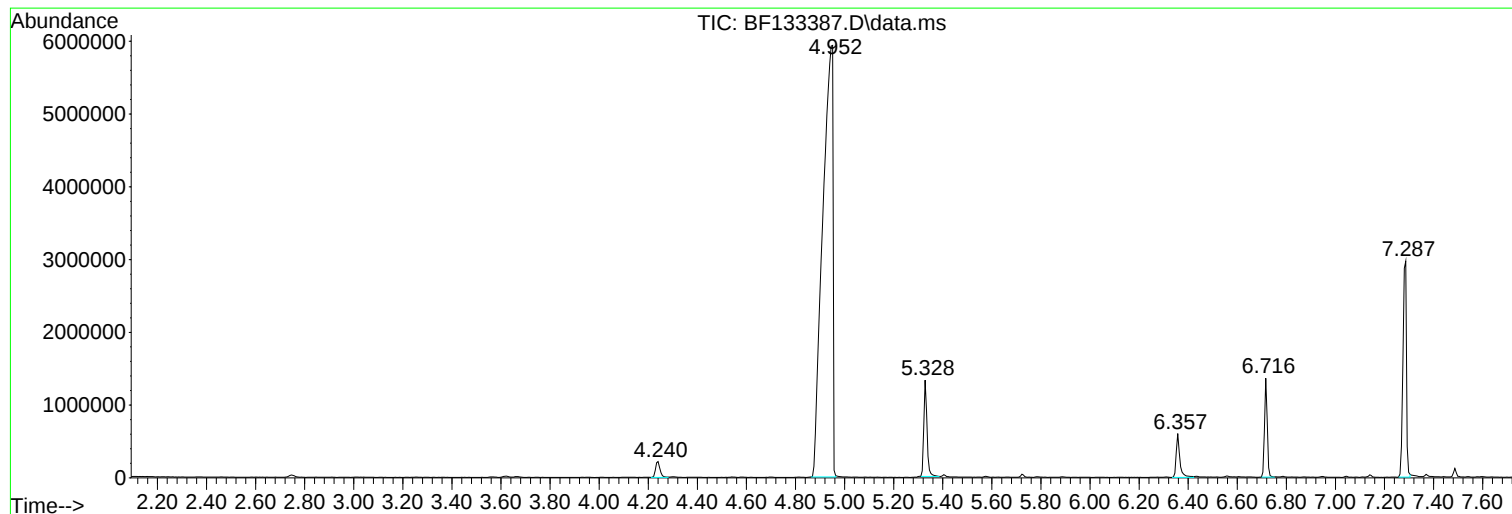
Sum of corrected areas: 42567093

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051523\
Data File : BF133387.D
Acq On : 15 May 2023 17:17
Operator : CG\JU
Sample : 02781-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP-WASTE-WASTER-5/12/23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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\BF051523\
Data File : BF133387.D
Acq On : 15 May 2023 17:17
Operator : CG\JU
Sample : 02781-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP-WASTE-WASTER-5/12/23

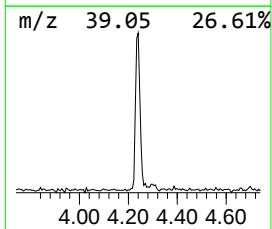
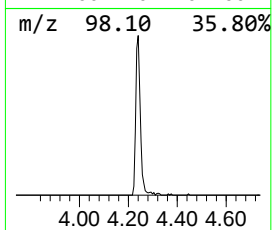
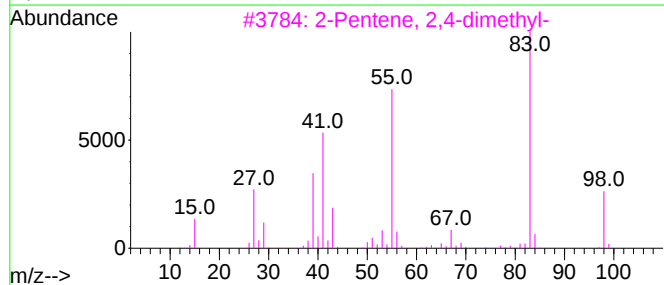
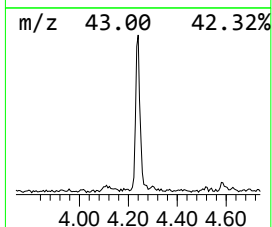
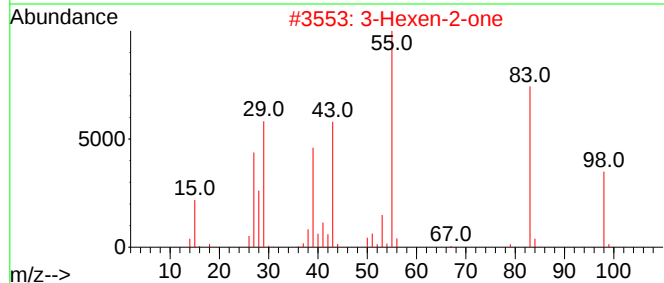
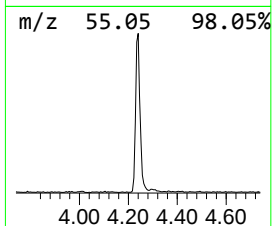
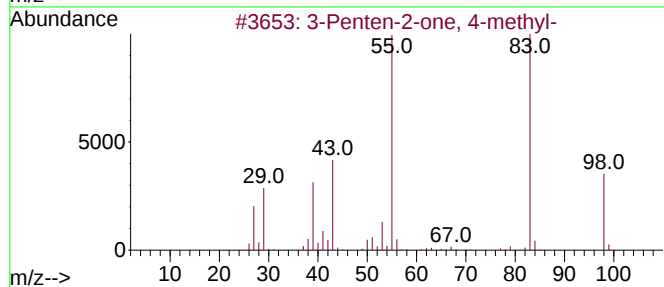
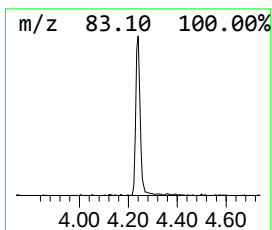
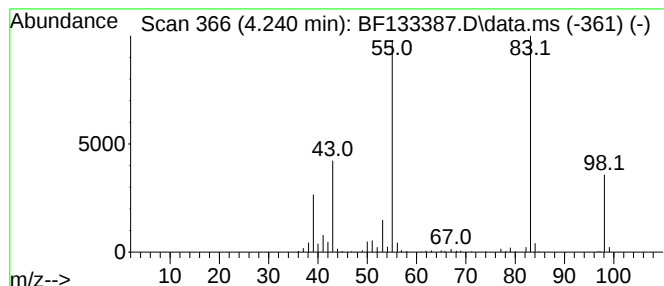
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.240	5.24 ng	275249	1,4-Dichlorobenzene-d4	6.716

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051523\
Data File : BF133387.D
Acq On : 15 May 2023 17:17
Operator : CG\JU
Sample : 02781-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

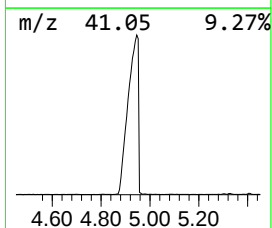
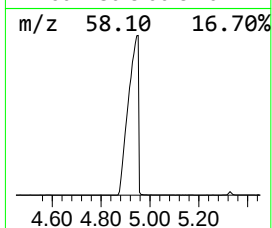
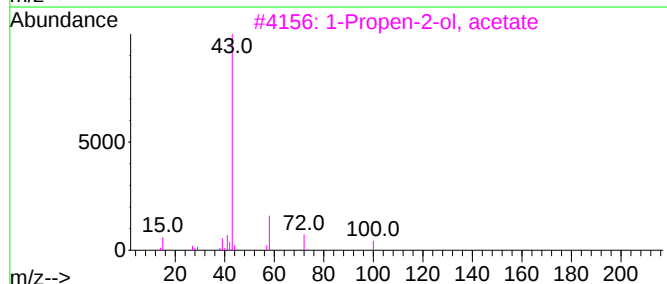
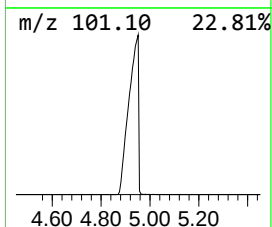
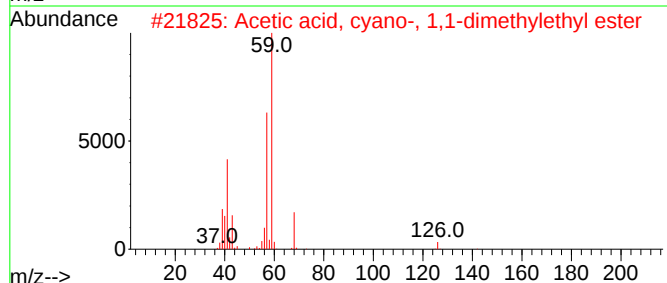
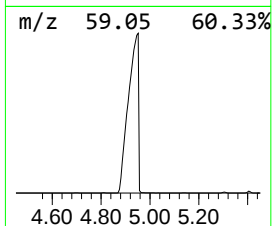
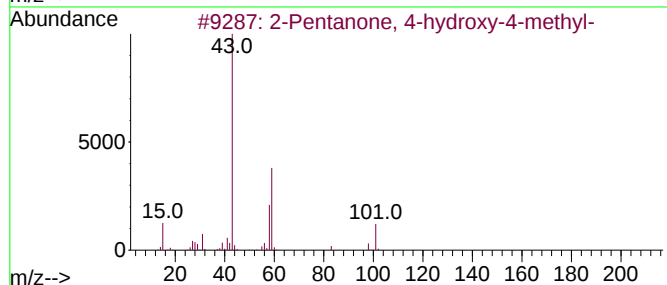
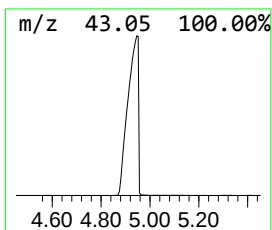
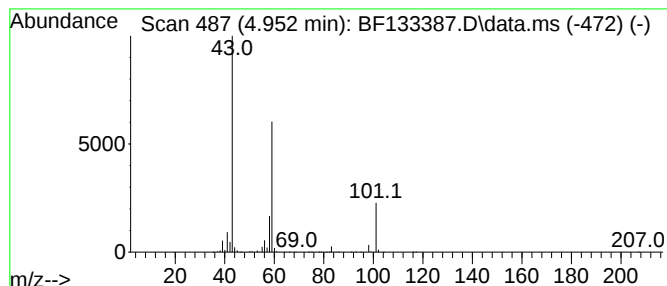
Instrument :
BNA_F
ClientSampleId :
MGP-WASTE-WASTER-5/12/23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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.	
4.952	329.88 ng	17339700	1,4-Dichlorobenzene-d4	6.716	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051523\
Data File : BF133387.D
Acq On : 15 May 2023 17:17
Operator : CG\JU
Sample : 02781-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP-WASTE-WASTER-5/12/23

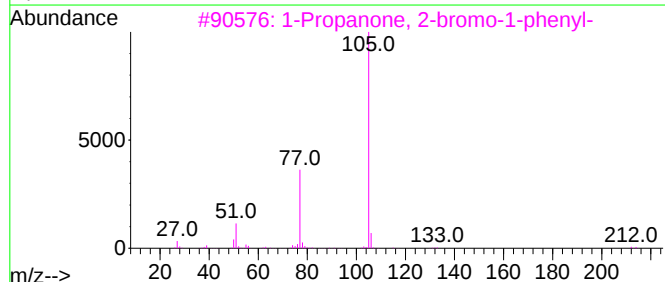
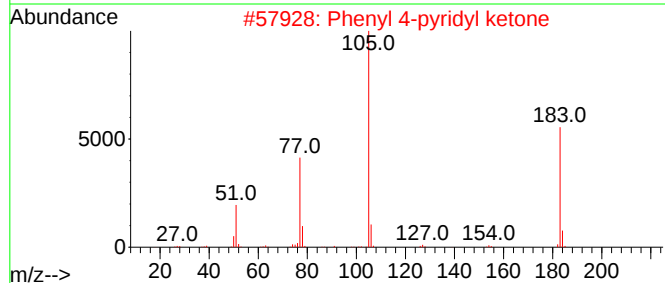
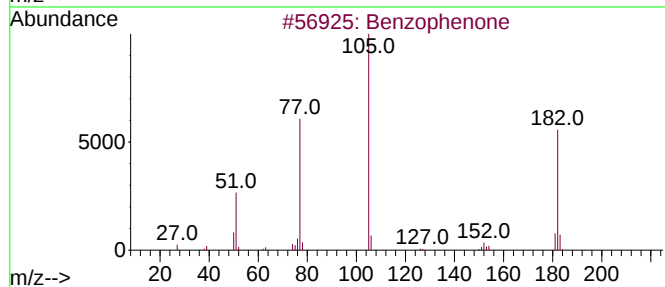
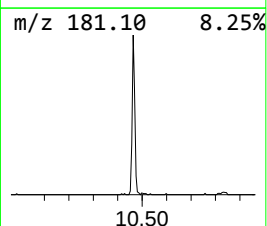
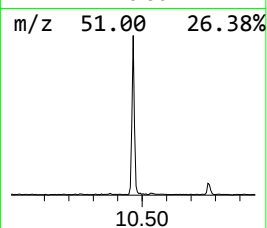
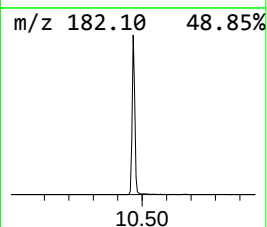
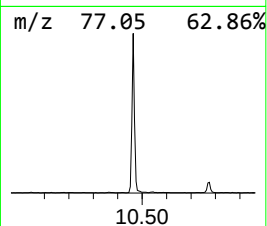
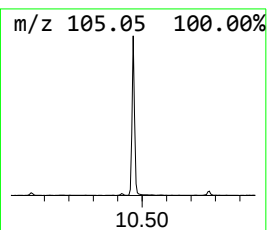
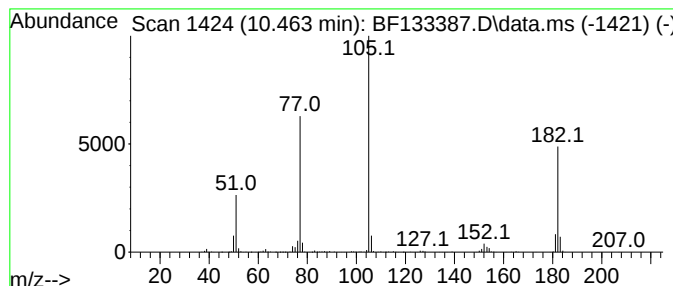
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.463	9.04 ng	704156	Acenaphthene-d10	9.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	52
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051523\
Data File : BF133387.D
Acq On : 15 May 2023 17:17
Operator : CG\JU
Sample : 02781-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP-WASTE-WASTER-5/12/23

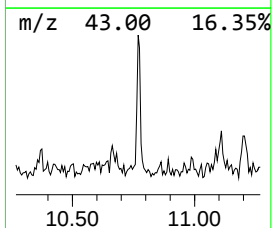
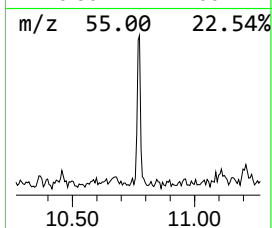
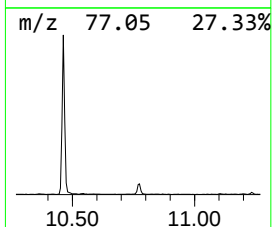
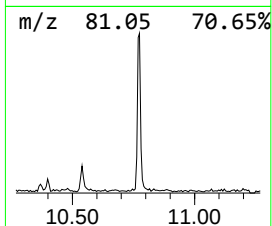
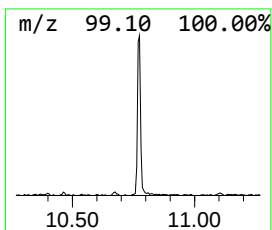
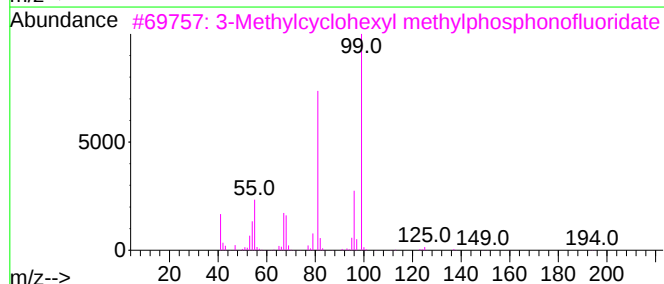
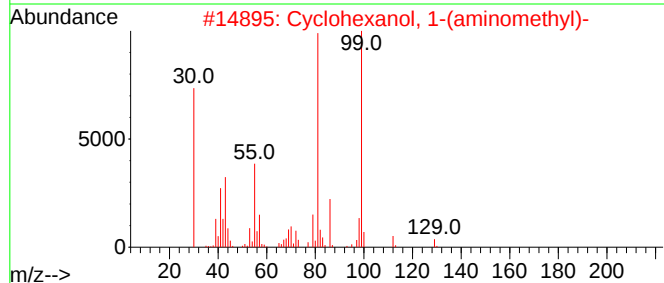
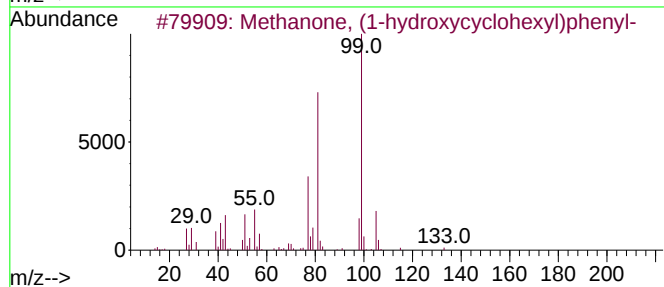
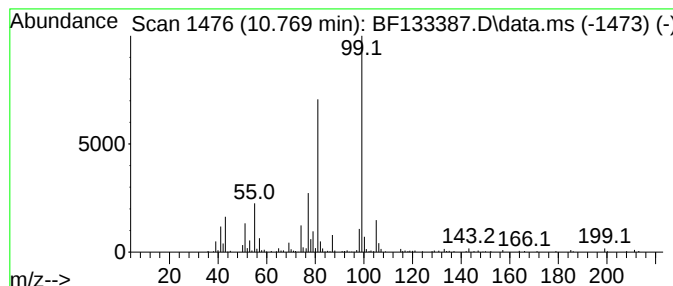
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.769	2.37 ng	177173	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	87
2			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	53
3			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	47
4			1-(Prop-2-yn-1-yl)cyclohexyl car...	181	C10H15NO2	000358-52-1	40
5			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051523\
Data File : BF133387.D
Acq On : 15 May 2023 17:17
Operator : CG\JU
Sample : 02781-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP-WASTE-WASTER-5/12/23

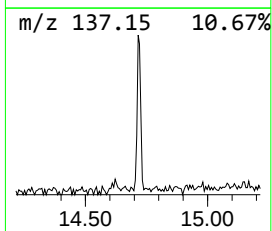
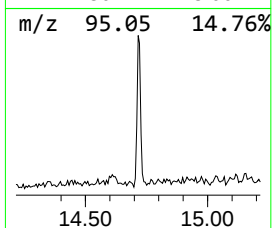
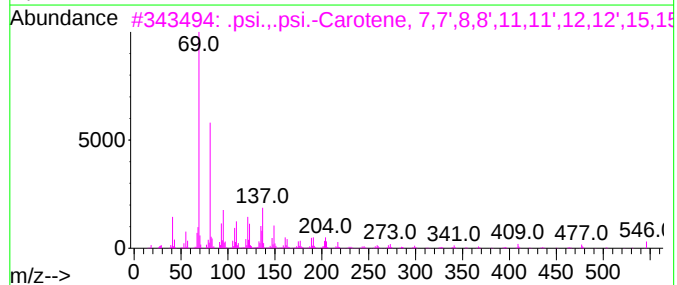
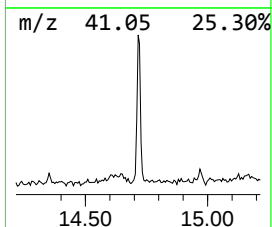
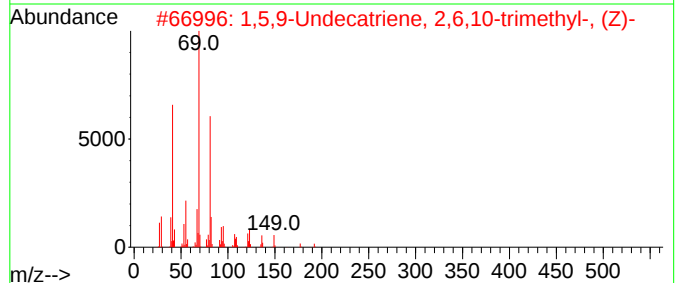
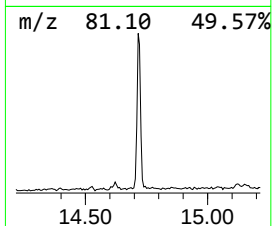
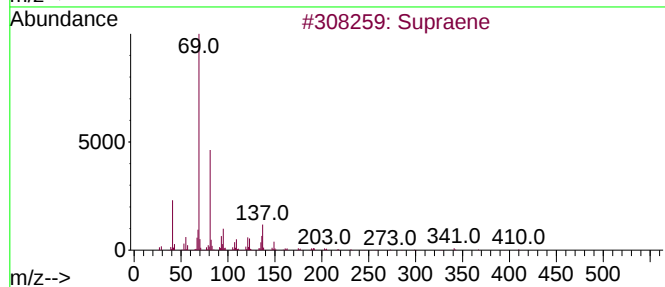
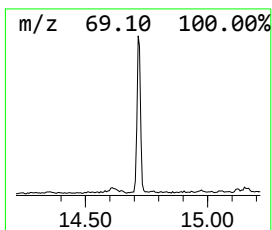
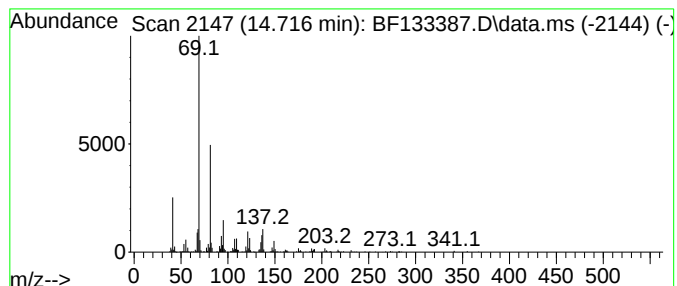
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.716	5.38 ng	295453	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	90
3			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4			(2E,6E,10E)-3,7,11,15-Tetramethy...	318	C21H34O2	125456-63-5	78
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051523\
Data File : BF133387.D
Acq On : 15 May 2023 17:17
Operator : CG\JU
Sample : 02781-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP-WASTE-WASTER-5/12/23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
3-Penten-2-one,...	4.240	5.2	ng	275249	1	6.716	1051280	20.0
2-Pentanone, 4-...	4.952	329.9	ng	17339700	1	6.716	1051280	20.0
Benzophenone	10.463	9.0	ng	704156	3	9.751	1557800	20.0
Methanone, (1-h...	10.769	2.4	ng	177173	4	11.233	1497840	20.0
Supraene	14.716	5.4	ng	295453	6	15.292	1099060	20.0