

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021822\
 Data File : BF126962.D
 Acq On : 18 Feb 2022 19:59
 Operator : CG\JU
 Sample : N1594-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-CONCRETE-COMP

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126962.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.710	235	242	257	rBV	206697	298601	2.46%	0.899%
2	4.592	379	392	395	rBV	5294511	12125341	100.00%	36.486%
3	5.181	483	492	495	rBV	2203312	3705077	30.56%	11.149%
4	5.545	551	554	561	rBV	313174	273711	2.26%	0.824%
5	6.545	720	724	736	rBV	1241373	1149288	9.48%	3.458%
6	6.928	786	789	793	rBV	765459	599047	4.94%	1.803%
7	7.251	840	844	847	rBV	543216	409071	3.37%	1.231%
8	7.492	877	885	888	rBV	1821468	1697113	14.00%	5.107%
9	8.104	986	989	993	rBV	206084	161068	1.33%	0.485%
10	8.210	1004	1007	1011	rBV	903187	753380	6.21%	2.267%
11	9.286	1185	1190	1193	rBV	3136387	2801242	23.10%	8.429%
12	9.363	1199	1203	1205	rBV2	376063	432516	3.57%	1.301%
13	9.398	1206	1209	1211	rVV3	218492	253192	2.09%	0.762%
14	9.604	1241	1244	1245	rBV2	358117	339392	2.80%	1.021%
15	9.627	1246	1248	1250	rVV	408498	378057	3.12%	1.138%
16	9.686	1254	1258	1260	rBV3	562561	828150	6.83%	2.492%
17	9.716	1260	1263	1265	rBV	1443786	1196173	9.87%	3.599%
18	9.839	1281	1284	1287	rBV3	882564	1267517	10.45%	3.814%
19	9.886	1289	1292	1294	rVV2	700272	850823	7.02%	2.560%
20	13.074	1832	1834	1842	rVB	1791710	1873277	15.45%	5.637%
21	14.121	2010	2012	2029	rVB	655408	1128331	9.31%	3.395%
22	15.615	2261	2266	2275	rVB	408938	542885	4.48%	1.634%
23	16.633	2436	2439	2449	rVB	94947	169764	1.40%	0.511%

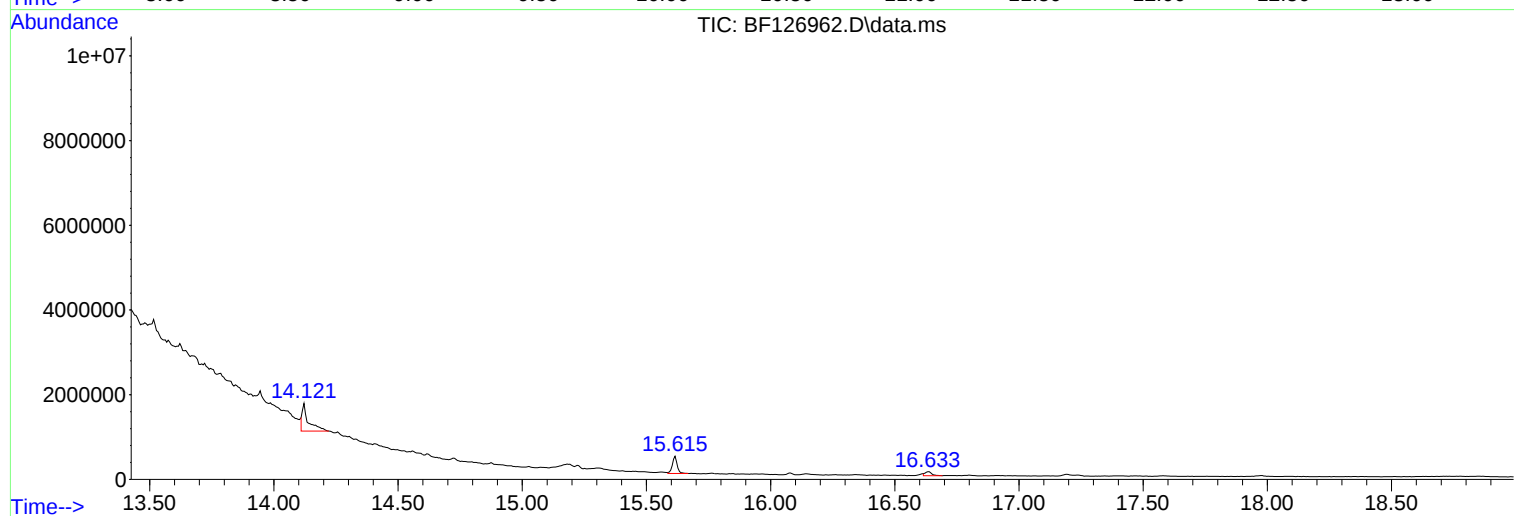
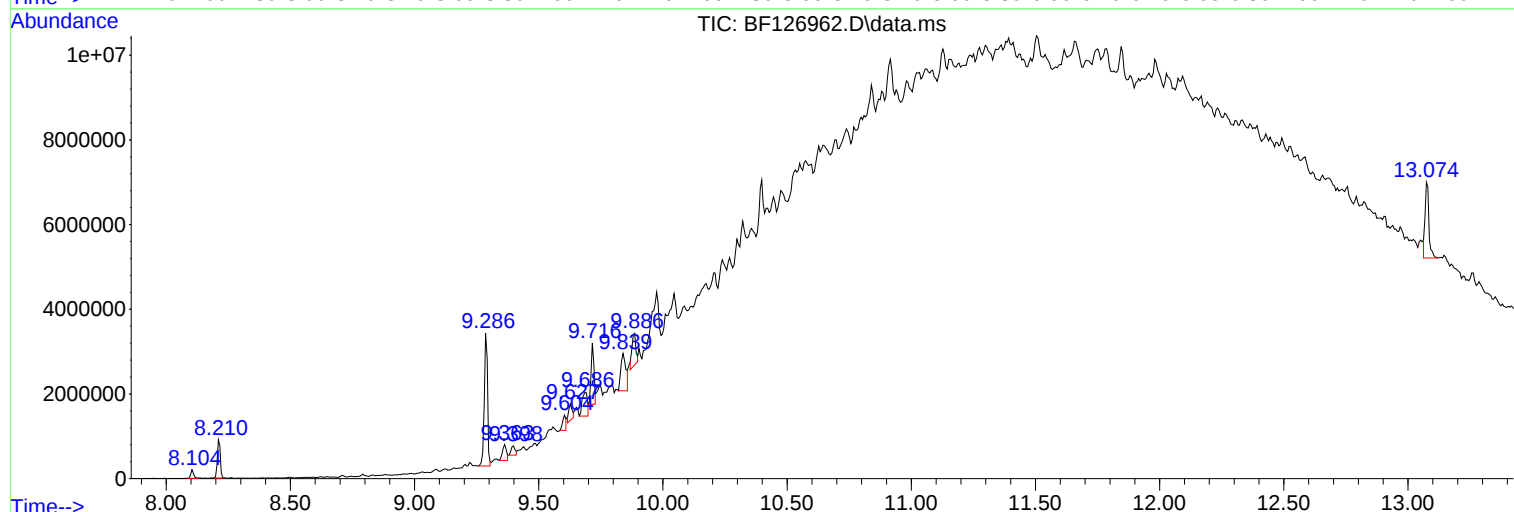
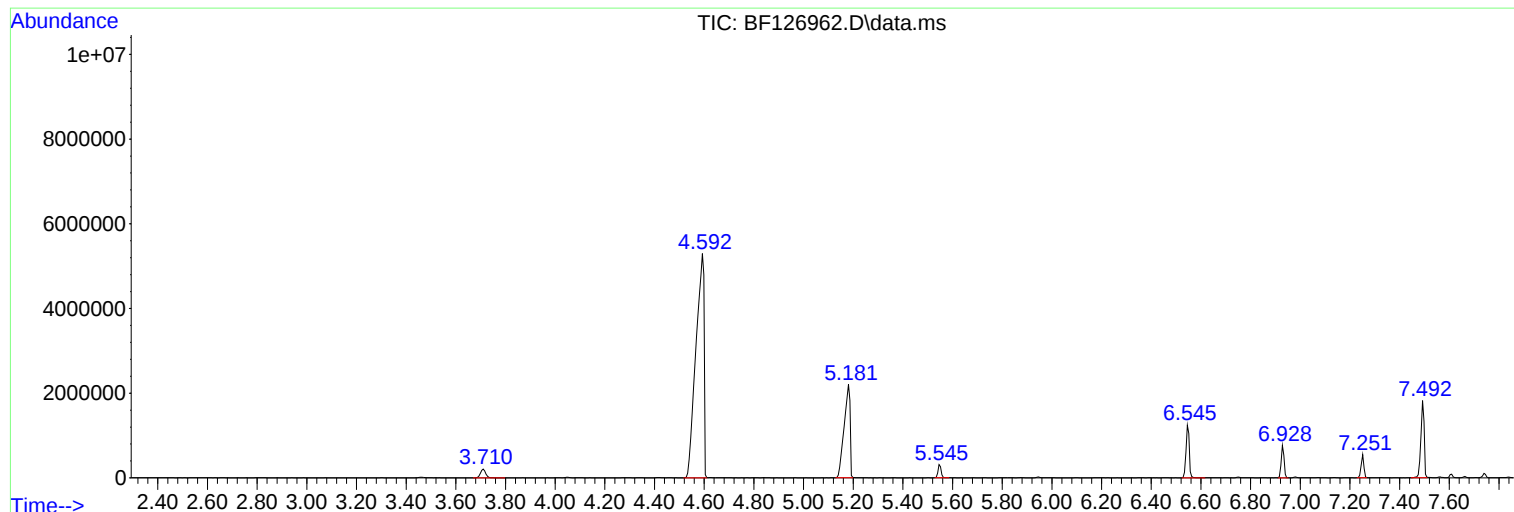
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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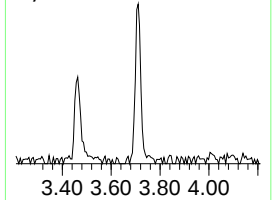
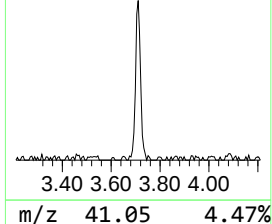
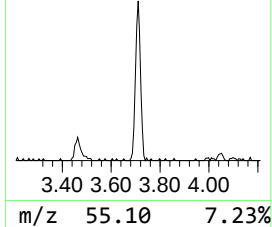
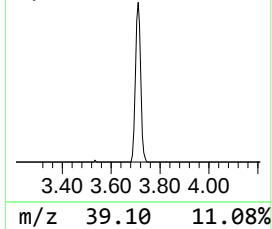
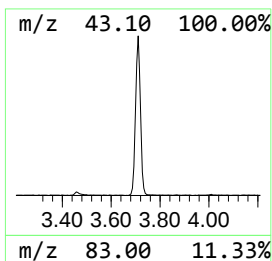
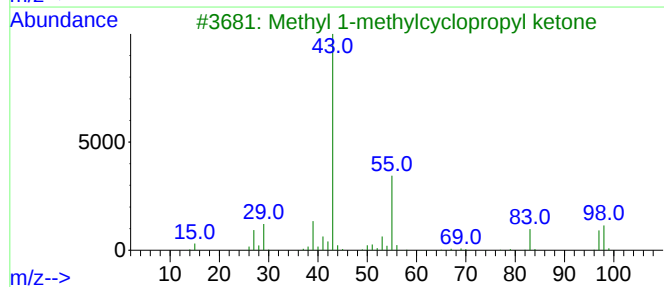
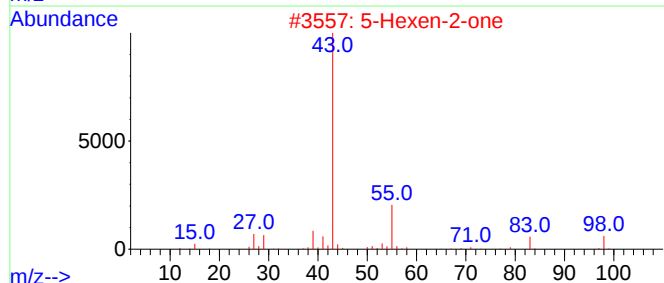
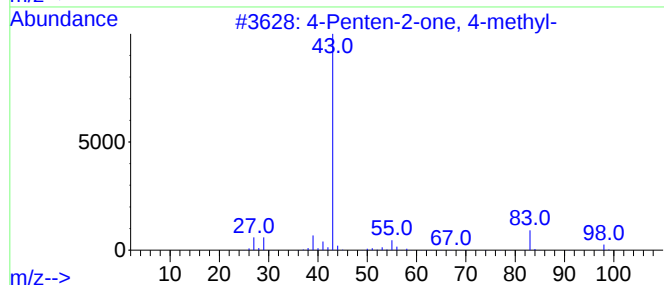
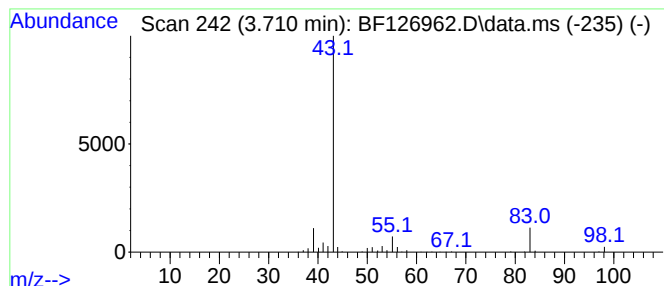
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.710	9.97 ng	298601	1,4-Dichlorobenzene-d4	6.928

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2		5-Hexen-2-one	98	C6H10O	000109-49-9	32
3		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	30
4		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	28
5		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17



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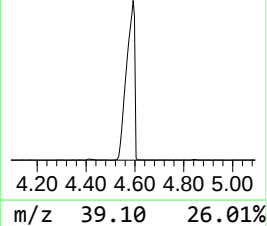
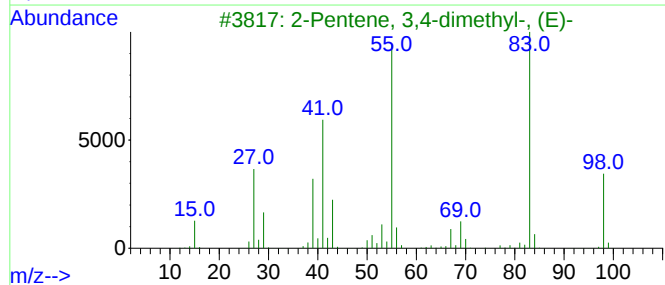
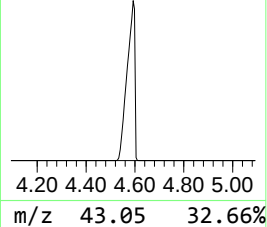
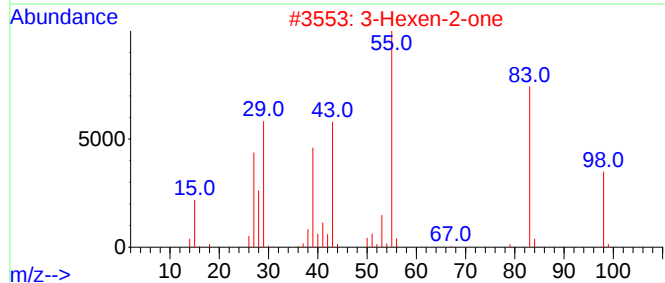
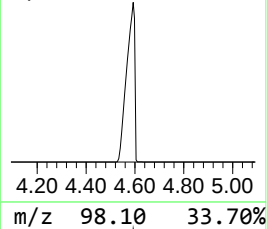
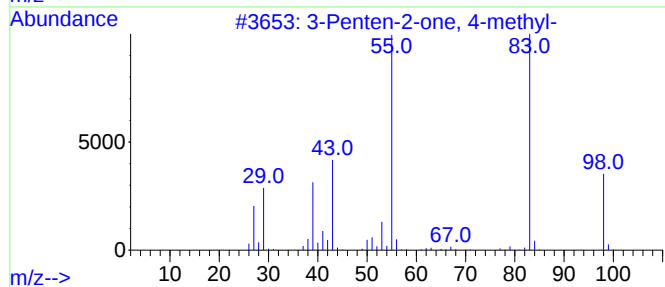
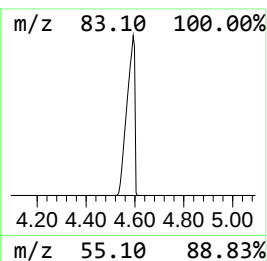
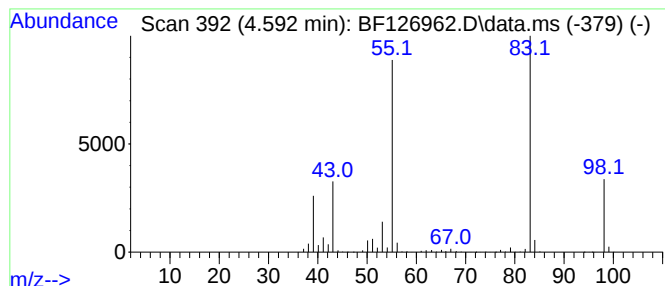
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.592	404.82 ng	12125300	1,4-Dichlorobenzene-d4	6.928

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, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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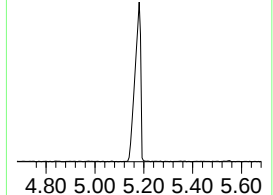
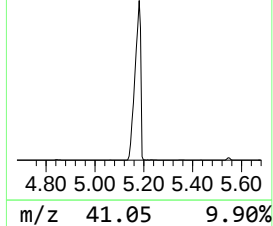
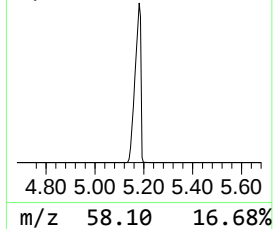
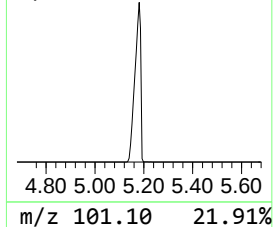
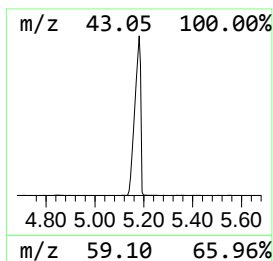
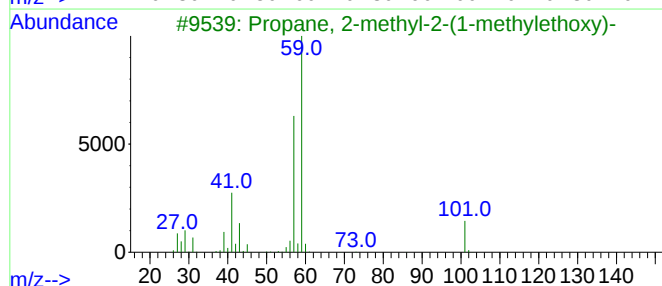
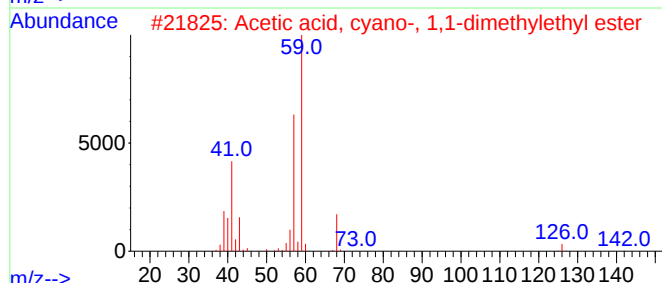
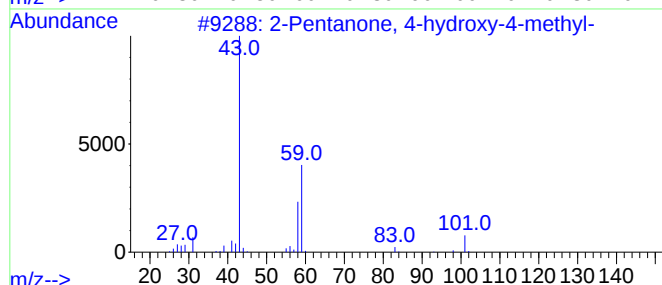
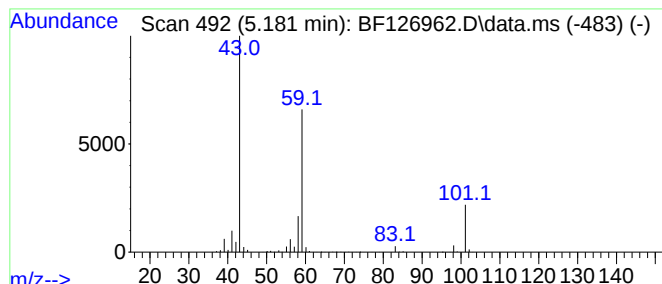
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	123.70 ng	3705080	1,4-Dichlorobenzene-d4	6.928

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	23
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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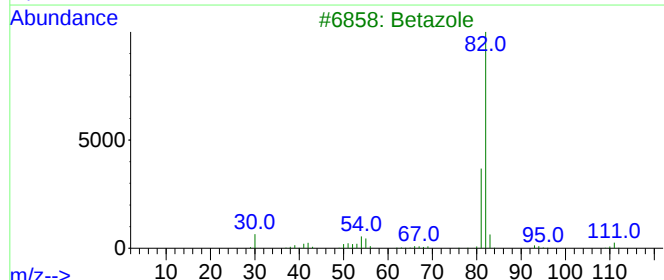
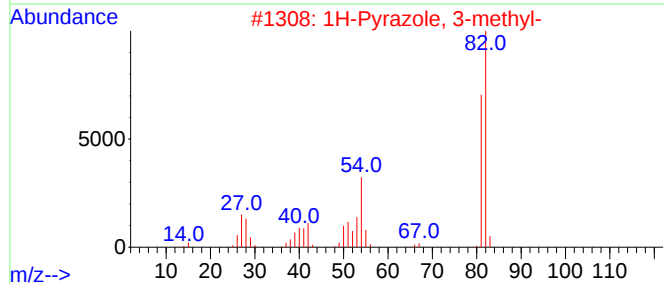
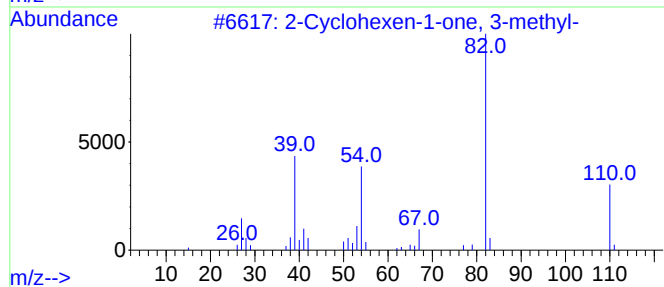
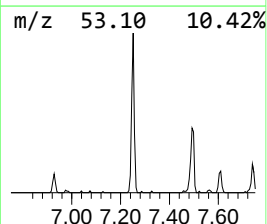
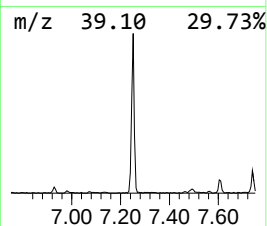
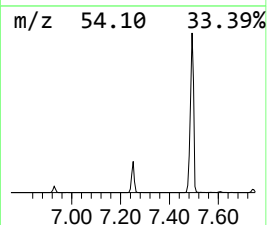
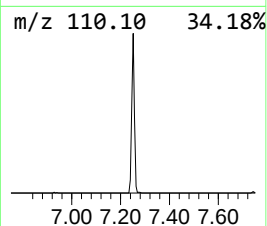
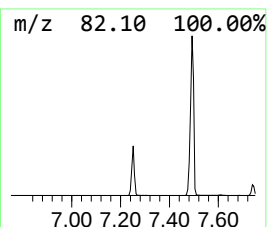
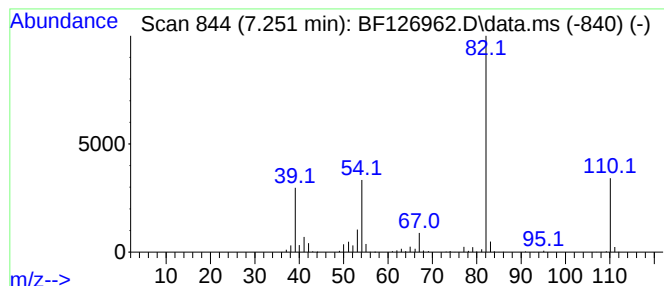
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Peak Number 4 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.251	13.66 ng	409071	1,4-Dichlorobenzene-d4	6.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2			1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	59
3			Betazole	111	C5H9N3	000105-20-4	40
4			1,2,3,6-Tetrahydropyridine	83	C5H9N	000694-05-3	38
5			1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	36



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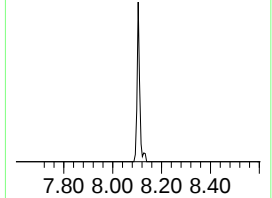
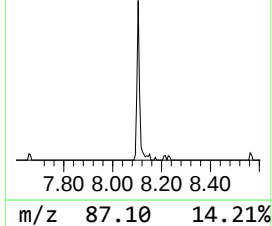
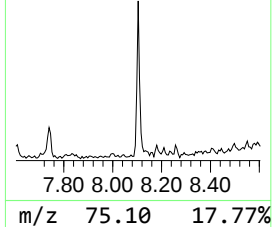
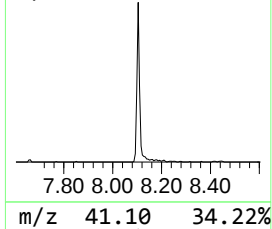
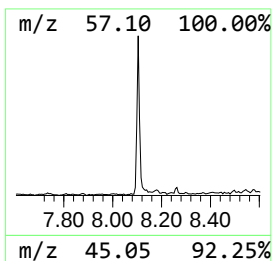
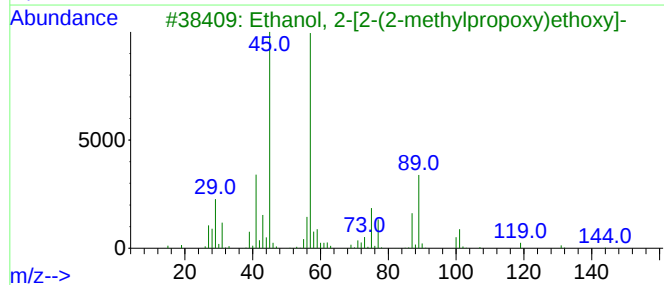
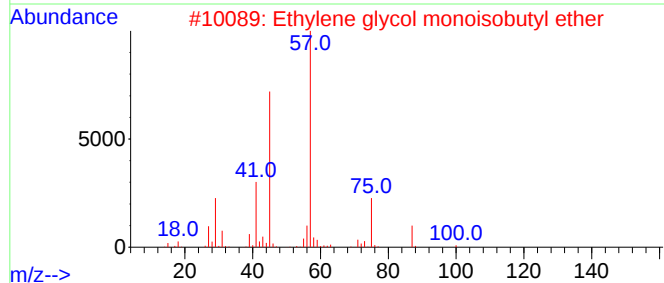
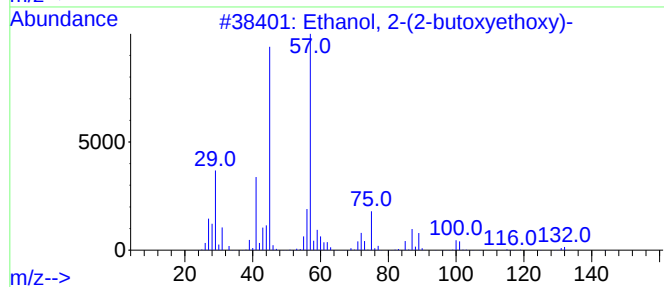
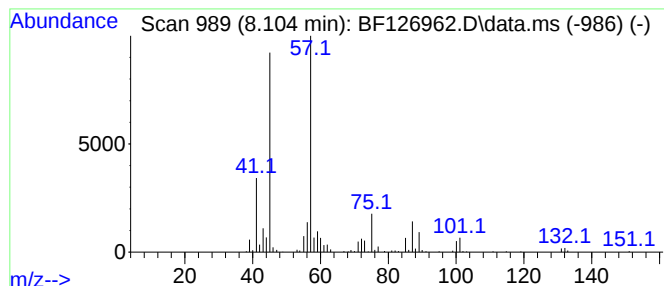
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	4.28 ng	161068	Naphthalene-d8	8.210

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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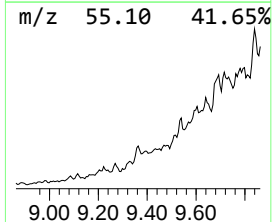
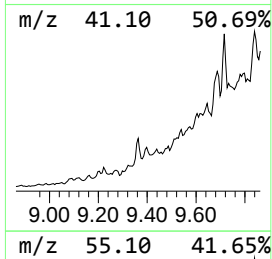
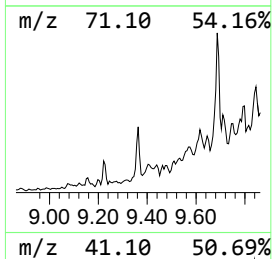
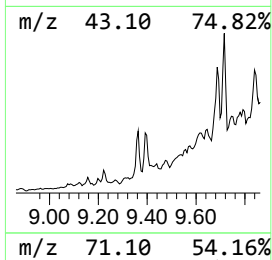
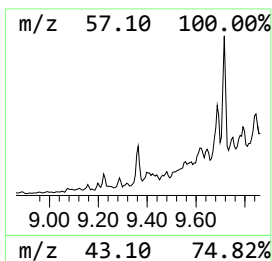
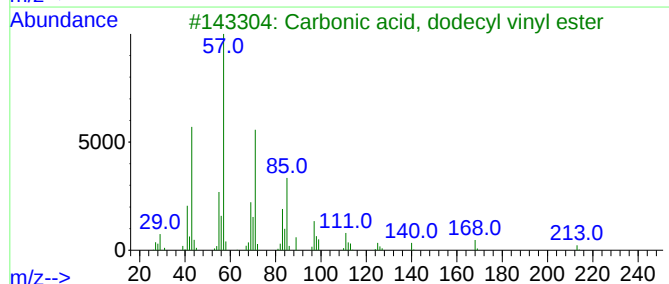
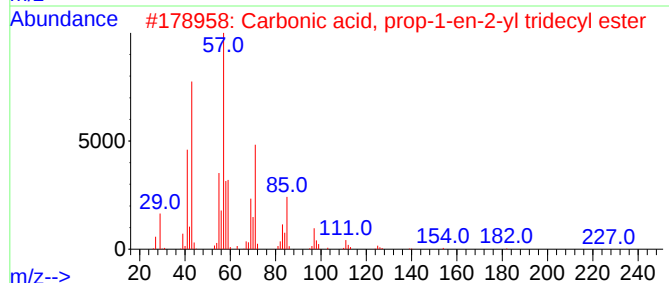
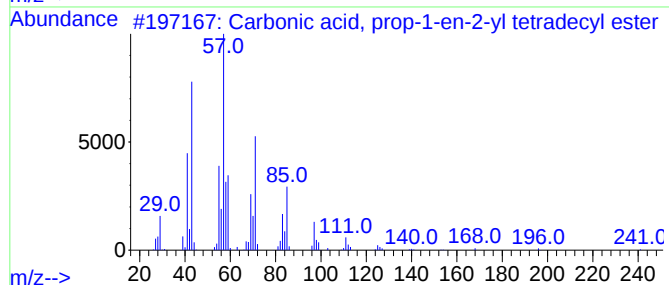
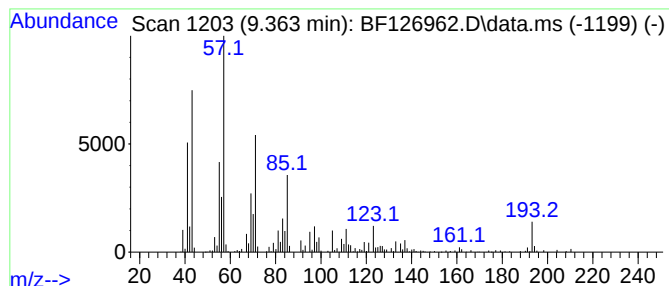
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Carbonic acid, prop-1-en-2-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.363	10.17 ng	432516	Acenaphthene-d10	9.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	81
2			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	68
3			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	64
4			Tetradecane	198	C14H30	000629-59-4	60
5			Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021822\
Data File : BF126962.D
Acq On : 18 Feb 2022 19:59
Operator : CG\JU
Sample : N1594-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

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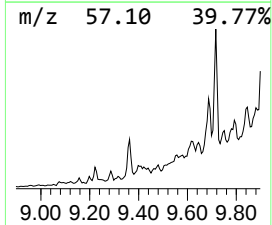
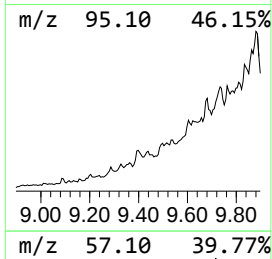
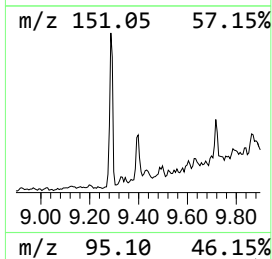
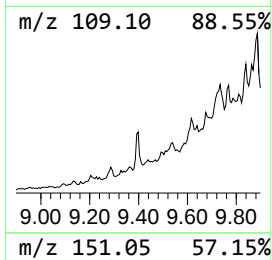
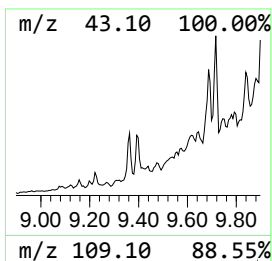
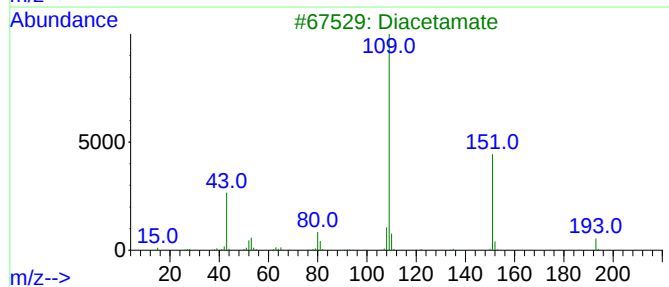
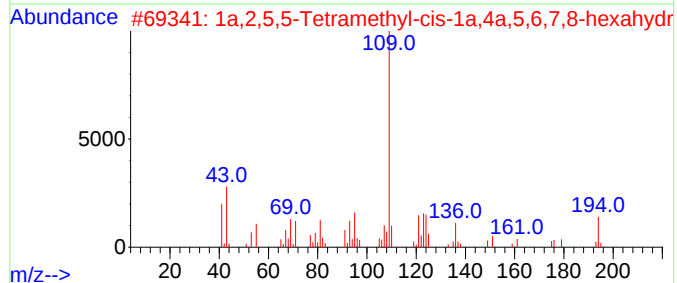
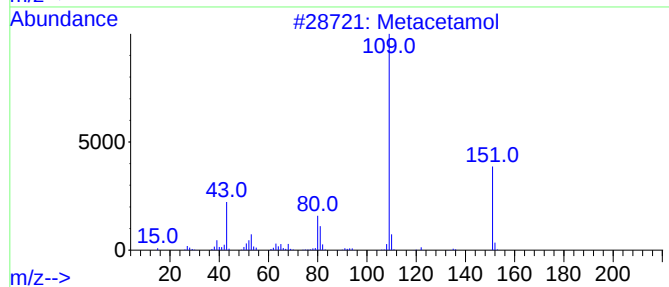
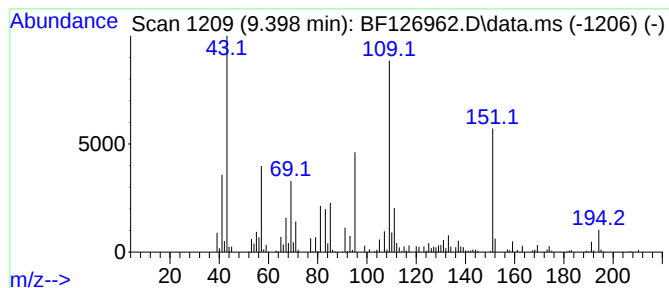
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.398 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.398	5.95 ng	253192	Acenaphthene-d10	9.974

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Metacetamol	151	C8H9NO2	000621-42-1	38
2		1a,2,5,5-Tetramethyl-cis-1a,4a,5...	194	C13H22O	1000215-77-7	38
3		Diacetamate	193	C10H11NO3	002623-33-8	38
4		Acetaminophen	151	C8H9NO2	000103-90-2	38
5		3-Fluorobenzyl isothiocyanate	167	C8H6FNS	063351-94-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021822\
Data File : BF126962.D
Acq On : 18 Feb 2022 19:59
Operator : CG\JU
Sample : N1594-01
Misc :
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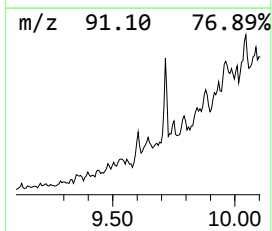
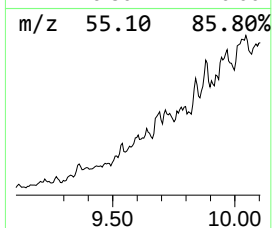
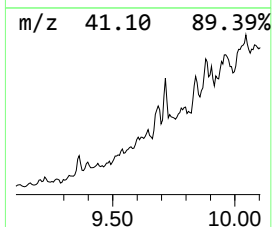
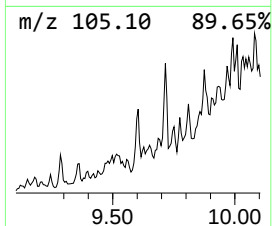
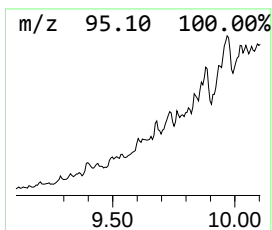
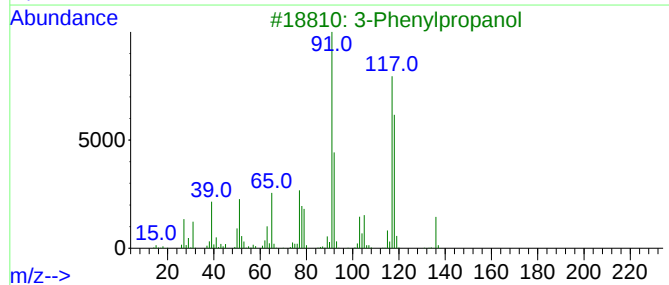
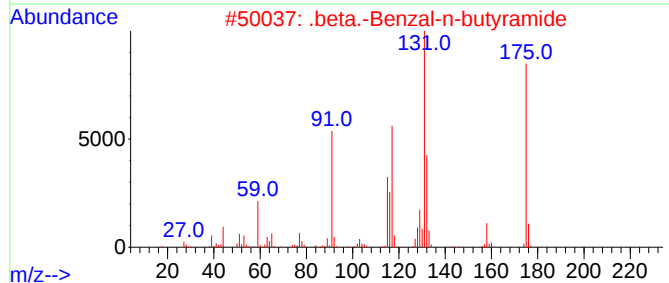
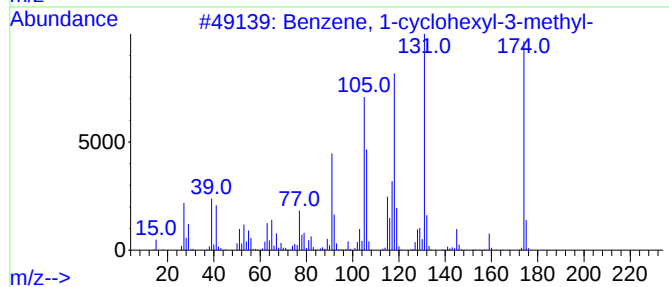
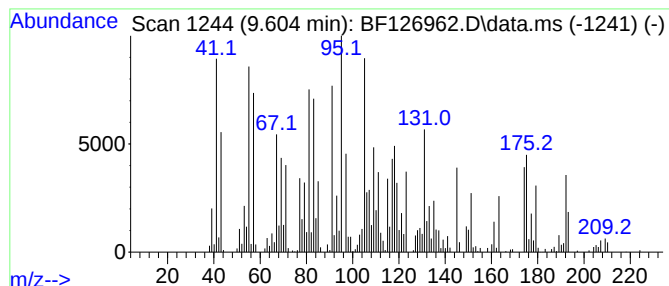
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.604 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.604	7.98 ng	339392	Acenaphthene-d10	9.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	35
2			.beta.-Benzal-n-butyramide	175	C11H13NO	007236-47-7	14
3			3-Phenylpropanol	136	C9H12O	000122-97-4	11
4			2H-Pyran-2-methanol, 3,4-dihydro...	192	C7H12O4S	067666-31-3	11
5			Isoborneol	154	C10H18O	000124-76-5	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021822\
Data File : BF126962.D
Acq On : 18 Feb 2022 19:59
Operator : CG\JU
Sample : N1594-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

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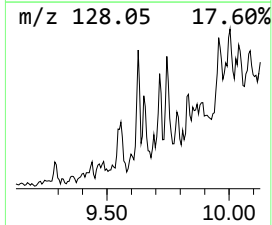
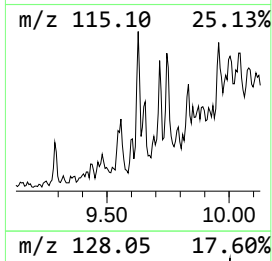
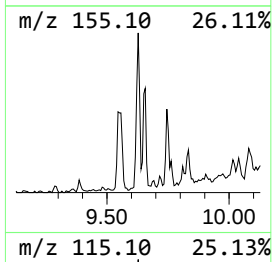
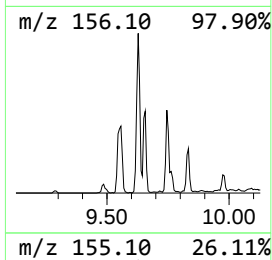
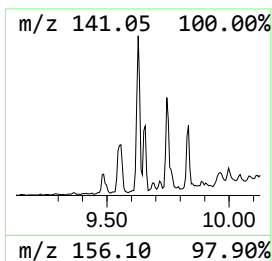
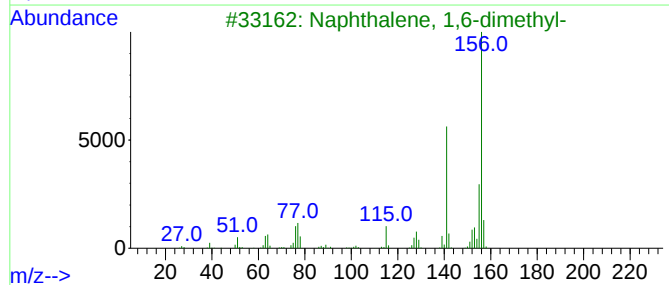
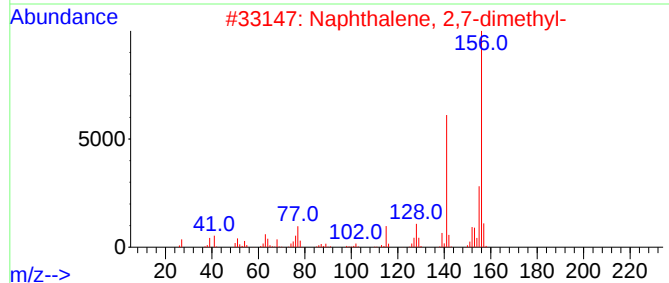
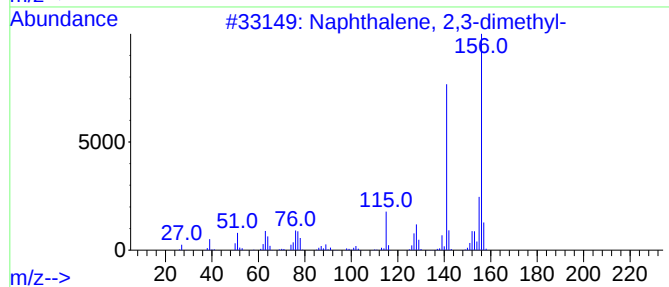
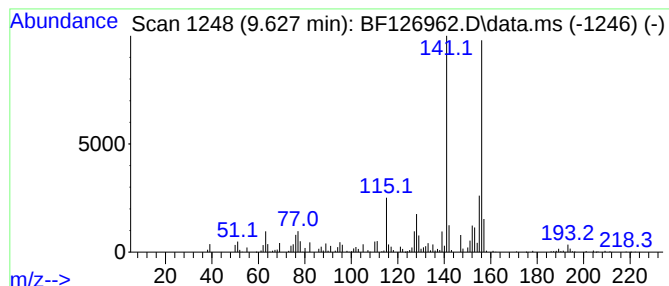
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.627	8.89 ng	378057	Acenaphthene-d10	9.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021822\
Data File : BF126962.D
Acq On : 18 Feb 2022 19:59
Operator : CG\JU
Sample : N1594-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

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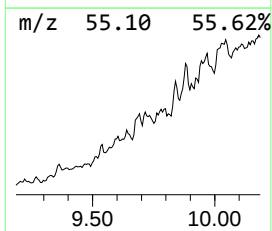
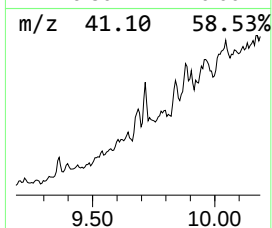
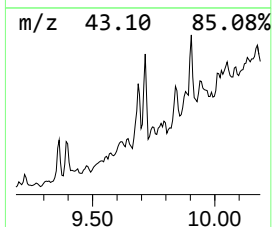
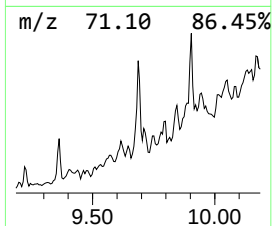
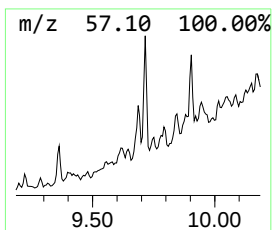
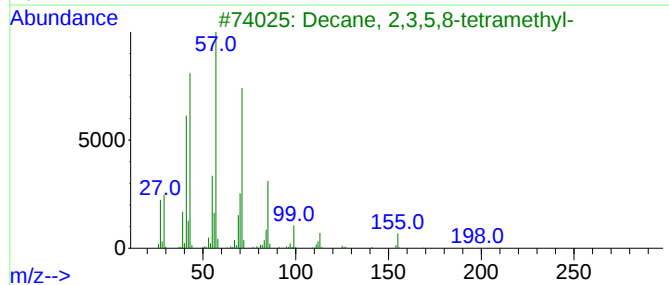
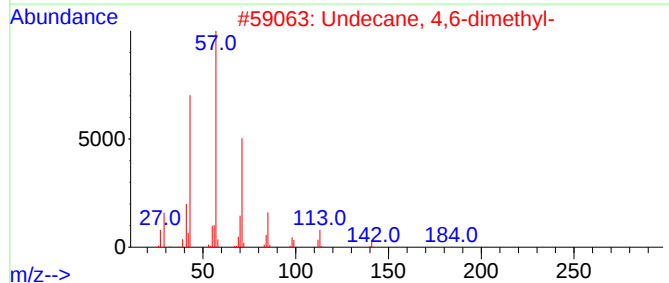
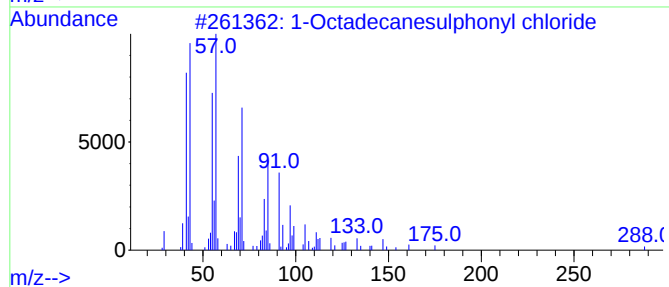
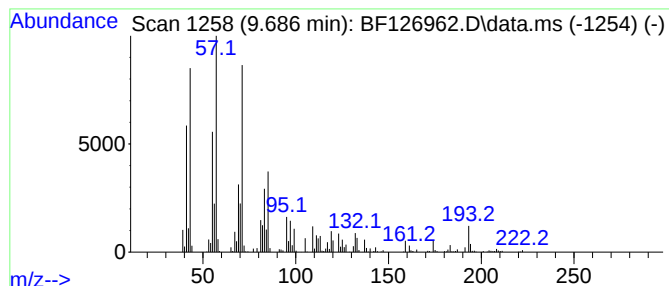
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Octadecanesulphonyl chloride Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.686	19.47 ng	828150	Acenaphthene-d10	9.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	64
2			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	52
3			Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	50
4			Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	47
5			Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021822\
Data File : BF126962.D
Acq On : 18 Feb 2022 19:59
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Instrument :
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ClientSampleId :
RO-CONCRETE-COMP

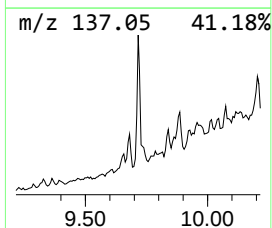
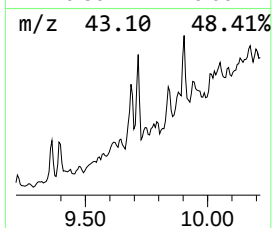
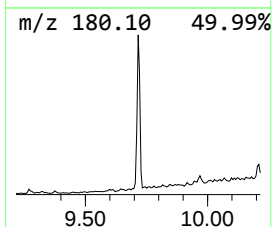
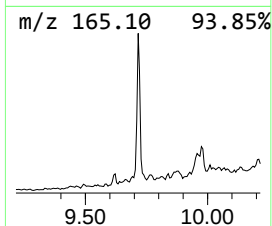
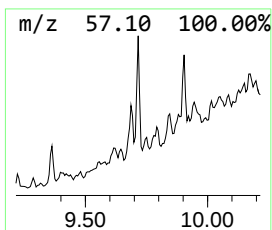
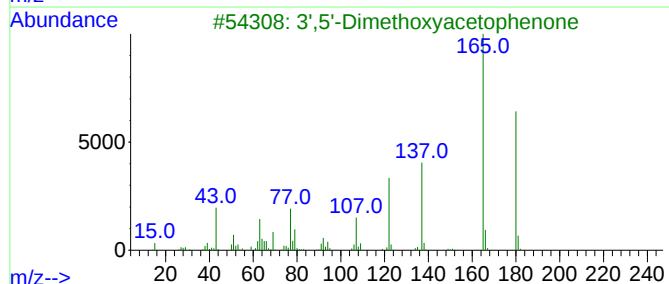
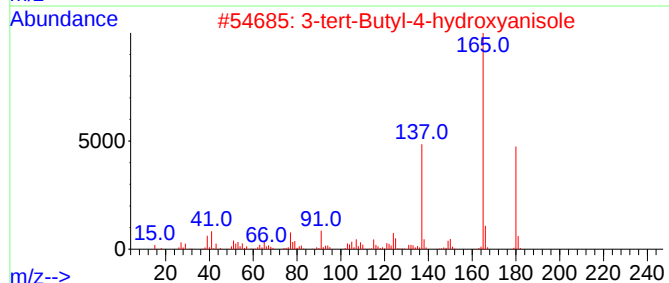
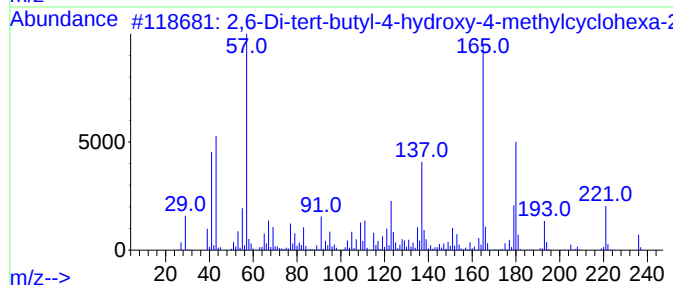
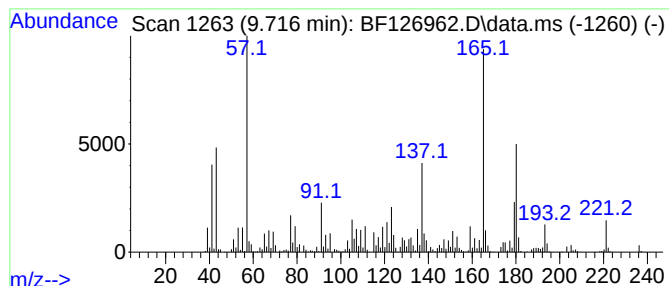
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2,6-Di-tert-butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.716	28.12 ng	1196170	Acenaphthene-d10	9.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Di-tert-butyl-4-hydroxy-4-me...	236	C15H24O2	010396-80-2	90		
2	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	62		
3	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	58		
4	Benzenamine, N-ethyl-N-methyl-4-...	180	C9H12N2O2	056269-48-8	55		
5	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	52		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021822\
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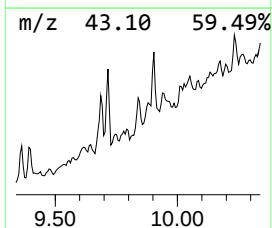
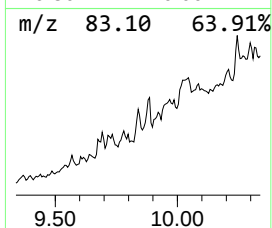
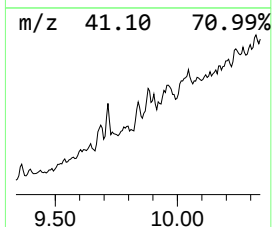
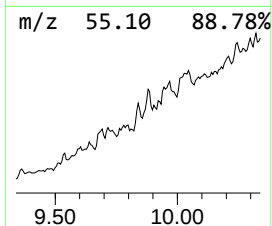
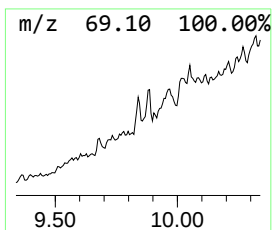
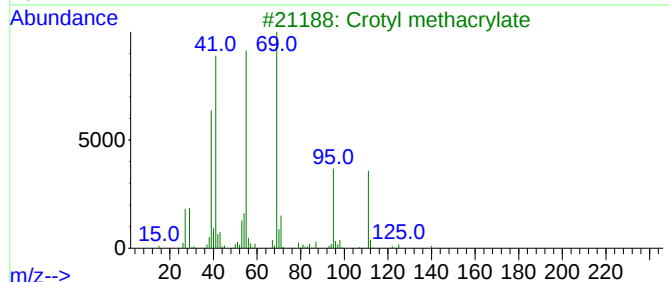
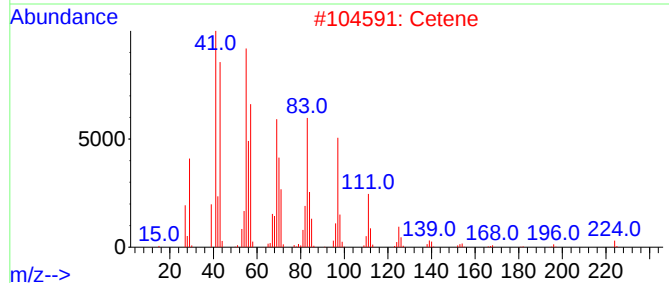
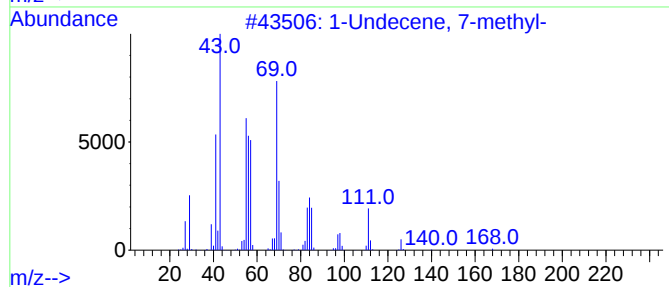
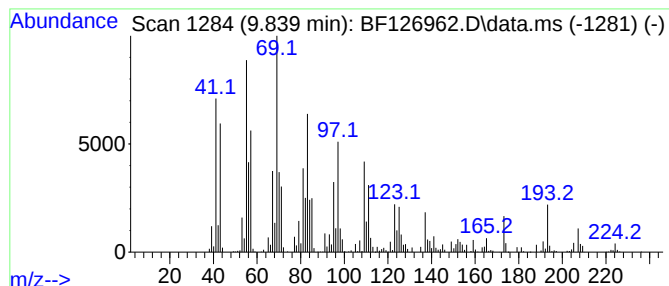
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown9.839 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.839	29.80 ng	1267520	Acenaphthene-d10	9.974

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1	Undecene, 7-methyl-	168	C12H24	074630-42-5	42
2	2	Cetene	224	C16H32	000629-73-2	35
3	3	Crotyl methacrylate	140	C8H12O2	007376-45-6	30
4	4	1-Hexadecanol	242	C16H34O	036653-82-4	30
5	5	1-Heptacosanol	396	C27H56O	002004-39-9	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021822\
Data File : BF126962.D
Acq On : 18 Feb 2022 19:59
Operator : CG\JU
Sample : N1594-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-CONCRETE-COMP

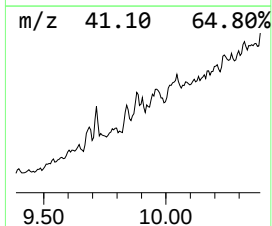
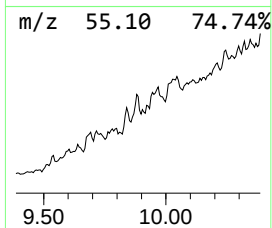
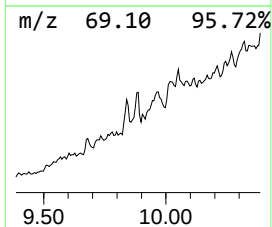
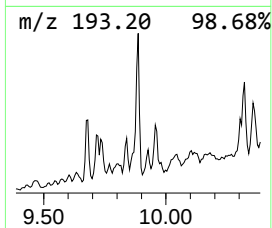
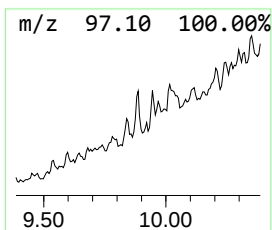
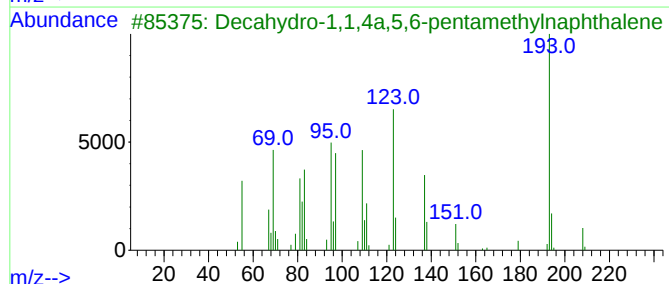
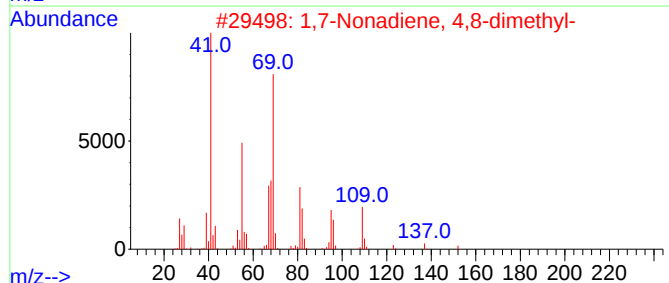
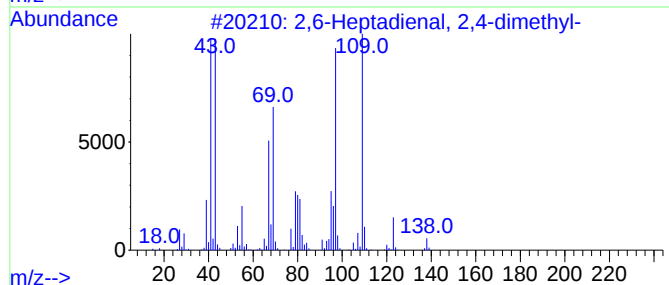
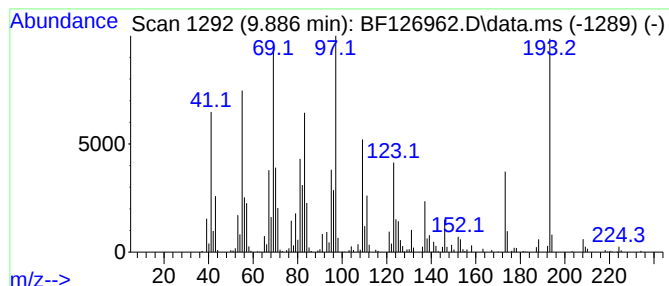
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown9.886 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.886	20.00 ng	850823	Acenaphthene-d10	9.974

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	43	
2	1,7-Nonadiene, 4,8-dimethyl-	152	C11H20	062108-28-5	41	
3	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	30	
4	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	30	
5	3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	27	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021822\
Data File : BF126962.D
Acq On : 18 Feb 2022 19:59
Operator : CG\JU
Sample : N1594-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-CONCRETE-COMP

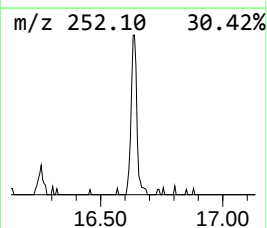
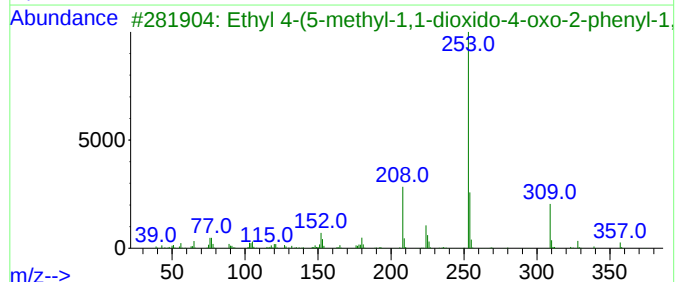
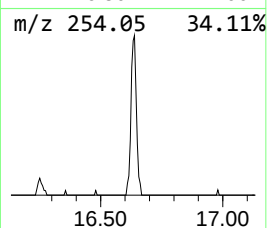
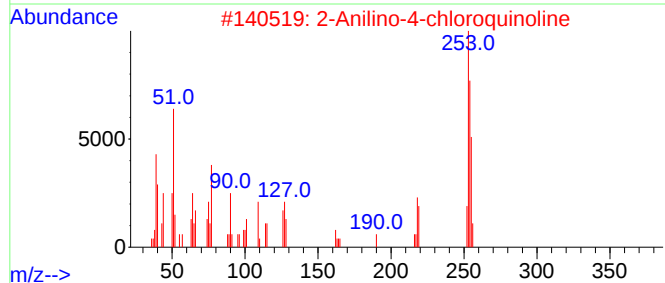
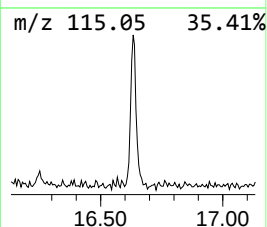
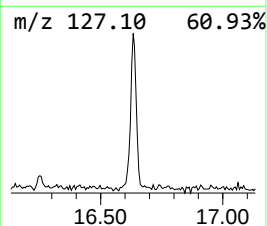
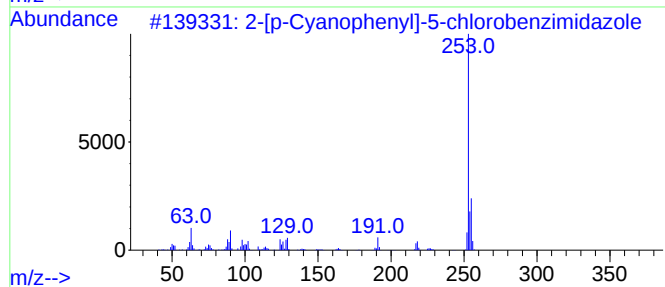
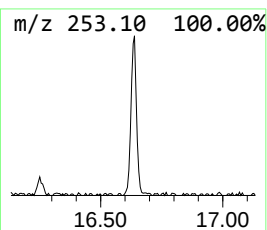
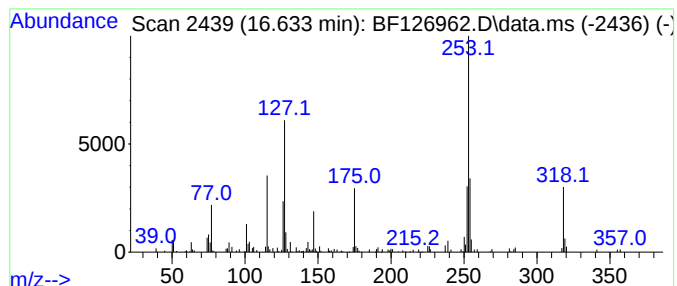
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown16.633 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.633	6.25 ng	169764	Perylene-d12	15.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2		[p-Cyanophenyl]-5-chlorobenzim...	253	C14H8ClN3	146132-86-7	27
2	2		Anilino-4-chloroquinoline	254	C15H11ClN2	032888-95-2	14
3	Ethyl	4-(5-methyl-1,1-dioxido-4-...	373	C19H19NO5S	1000294-64-6	12	
4	1,1-Dioxido-1,2-benzisothiazol-3...	254	C10H14N2O2SSi	1000479-94-7	12		
5	6-Chloro-2-methyl-4-phenyl-quino...	253	C16H12ClN	022609-12-7	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021822\
Data File : BF126962.D
Acq On : 18 Feb 2022 19:59
Operator : CG\JU
Sample : N1594-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-CONCRETE-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one,...	3.710	10.0	ng	298601	1	6.928	599047	20.0
3-Penten-2-one,...	4.592	404.8	ng	12125300	1	6.928	599047	20.0
2-Pentanone, 4-...	5.181	123.7	ng	3705080	1	6.928	599047	20.0
2-Cyclohexen-1-...	7.251	13.7	ng	409071	1	6.928	599047	20.0
Ethanol, 2-(2-b...	8.104	4.3	ng	161068	2	8.210	753380	20.0
Carbonic acid, ...	9.363	10.2	ng	432516	3	9.974	850823	20.0
unknown9.398	9.398	6.0	ng	253192	3	9.974	850823	20.0
unknown9.604	9.604	8.0	ng	339392	3	9.974	850823	20.0
Naphthalene, 2,...	9.627	8.9	ng	378057	3	9.974	850823	20.0
1-Octadecanesul...	9.686	19.5	ng	828150	3	9.974	850823	20.0
2,6-Di-tert-but...	9.716	28.1	ng	1196170	3	9.974	850823	20.0
unknown9.839	9.839	29.8	ng	1267520	3	9.974	850823	20.0
unknown9.886	9.886	20.0	ng	850823	3	9.974	850823	20.0
unknown16.633	16.633	6.3	ng	169764	6	15.615	542885	20.0