

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
 Data File : BF130321.D
 Acq On : 19 Sep 2022 15:19
 Operator : CG\JU
 Sample : N4656-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130321.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.845	465	469	480	rVB	84173	110334	4.71%	0.638%
2	5.263	535	540	543	rBV	1928527	1851860	78.98%	10.703%
3	6.292	710	715	718	rBV	1834522	1884584	80.37%	10.892%
4	6.657	774	777	781	rVB	725234	568805	24.26%	3.287%
5	7.222	868	873	876	rBV	1284337	1251670	53.38%	7.234%
6	7.851	977	980	991	rBV	395857	545726	23.27%	3.154%
7	7.939	991	995	998	rVB	905810	747188	31.87%	4.318%
8	9.016	1173	1178	1181	rBV	2884297	2344743	100.00%	13.551%
9	9.139	1195	1199	1210	rVB	291209	285798	12.19%	1.652%
10	9.686	1288	1292	1296	rBV	981212	814765	34.75%	4.709%
11	10.475	1418	1426	1429	rBV	1577191	1440515	61.44%	8.325%
12	11.169	1540	1544	1546	rBV	813029	737732	31.46%	4.264%
13	11.186	1546	1547	1551	rVV	54945	38627	1.65%	0.223%
14	11.239	1551	1556	1559	rVB	38094	36590	1.56%	0.211%
15	11.392	1578	1582	1591	rVB	35243	50957	2.17%	0.295%
16	11.574	1609	1613	1616	rVB	76706	66027	2.82%	0.382%
17	11.704	1630	1635	1637	rBV2	54338	56472	2.41%	0.326%
18	11.733	1637	1640	1644	rVB	36238	48719	2.08%	0.282%
19	12.274	1729	1732	1738	rVB	206863	184644	7.87%	1.067%
20	12.363	1744	1747	1753	rVB2	146939	170987	7.29%	0.988%
21	12.592	1780	1786	1790	rBV	81808	118074	5.04%	0.682%
22	12.751	1808	1813	1817	rBV	2037506	1789514	76.32%	10.342%
23	13.204	1888	1890	1892	rBV	40870	35527	1.52%	0.205%
24	13.233	1892	1895	1901	rVB	93856	104271	4.45%	0.603%
25	13.298	1903	1906	1910	rBV	42739	45567	1.94%	0.263%
26	13.792	1972	1990	1993	rBV2	664909	846913	36.12%	4.895%
27	13.815	1993	1994	2005	rVB	135059	119212	5.08%	0.689%
28	14.404	2090	2094	2097	rVB	71952	65716	2.80%	0.380%
29	14.792	2156	2160	2162	rBV	68107	80869	3.45%	0.467%
30	14.815	2162	2164	2168	rVV	54248	57158	2.44%	0.330%
31	14.880	2172	2175	2182	rVB2	28772	31714	1.35%	0.183%
32	15.121	2213	2216	2221	rVB	33647	41720	1.78%	0.241%
33	15.180	2222	2226	2231	rBV	420597	495536	21.13%	2.864%
34	15.621	2297	2301	2308	rVB2	28361	43809	1.87%	0.253%
35	16.656	2472	2477	2485	rVB6	70951	129143	5.51%	0.746%
36	18.898	2852	2858	2865	rVB6	23298	61254	2.61%	0.354%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130321.D
Acq On : 19 Sep 2022 15:19
Operator : CG\JU
Sample : N4656-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

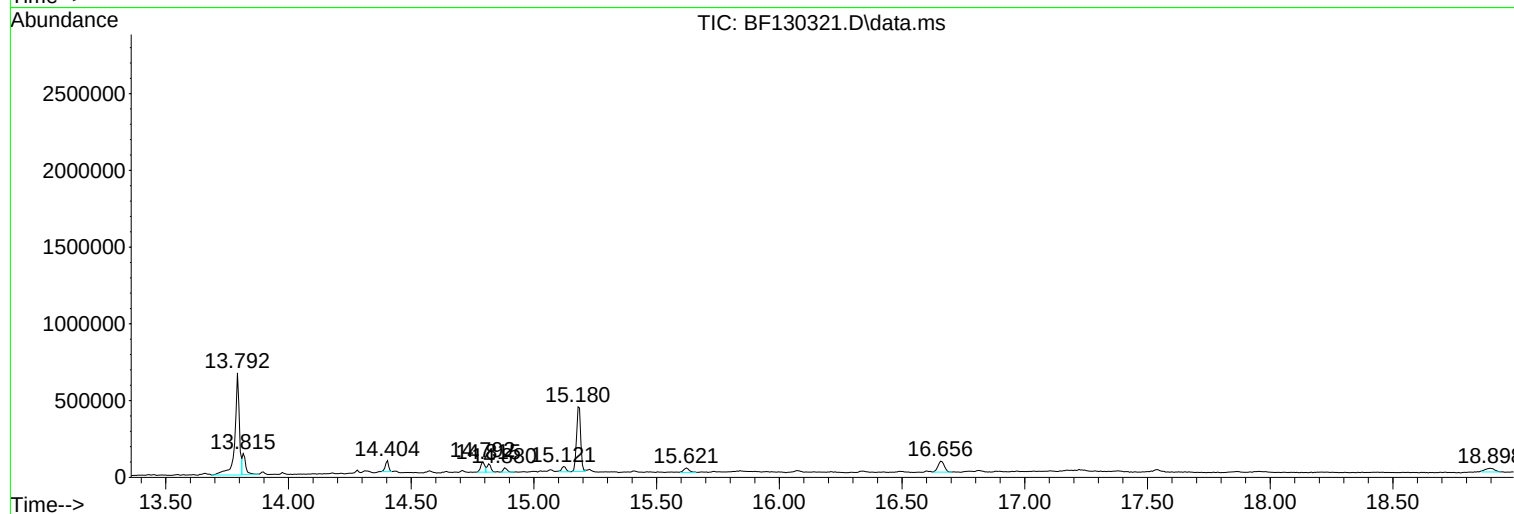
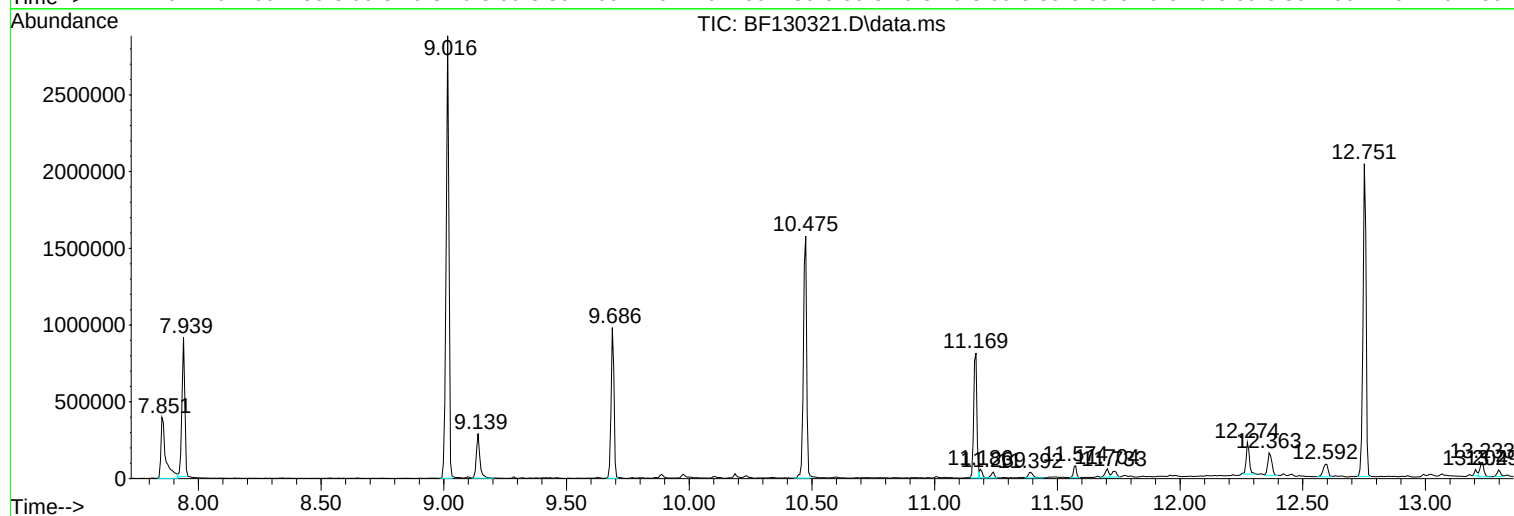
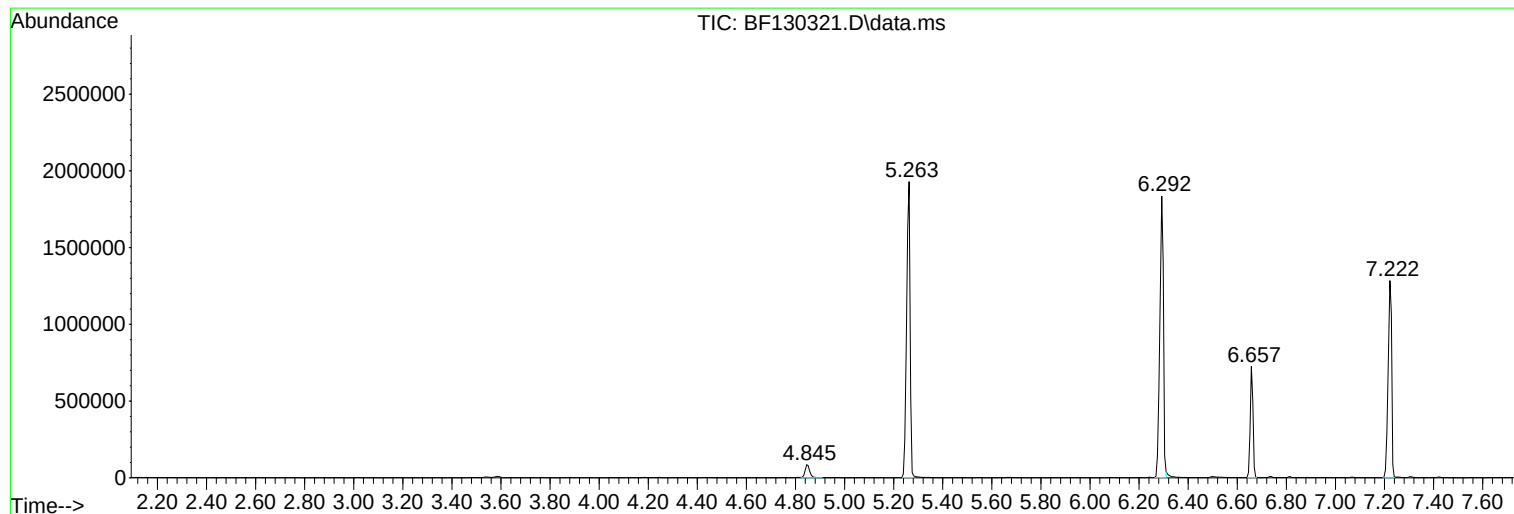
Sum of corrected areas: 17302740

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130321.D
Acq On : 19 Sep 2022 15:19
Operator : CG\JU
Sample : N4656-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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\BF091922\
Data File : BF130321.D
Acq On : 19 Sep 2022 15:19
Operator : CG\JU
Sample : N4656-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

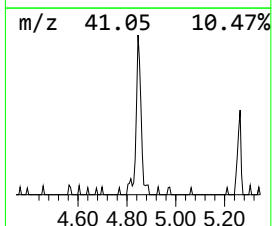
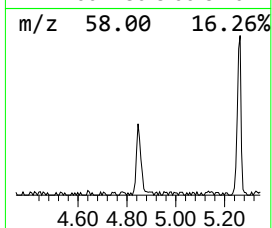
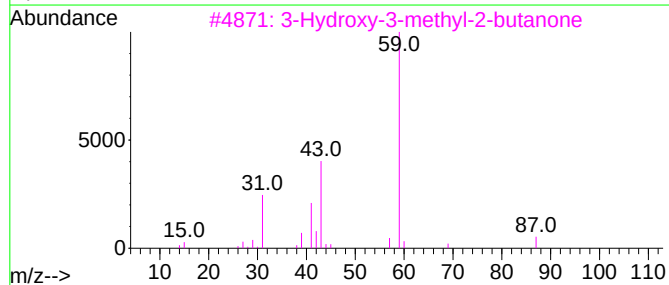
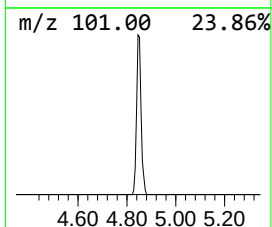
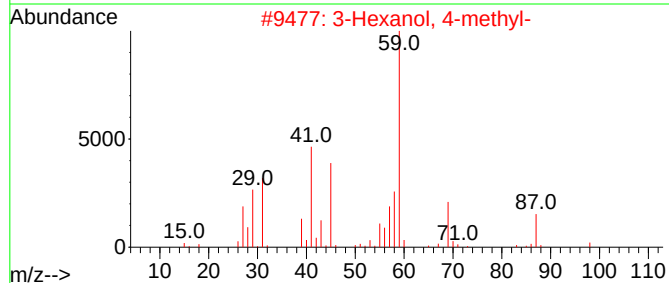
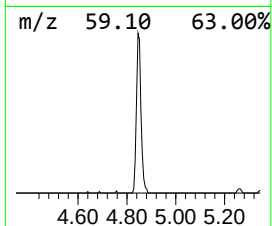
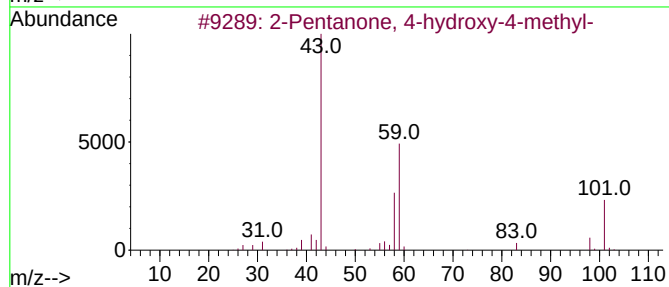
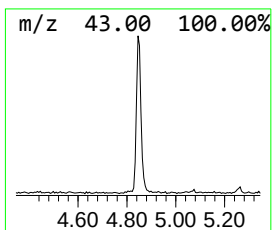
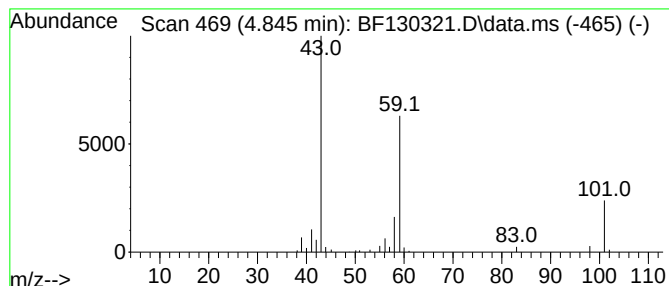
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.845	3.88 ng	110334	1,4-Dichlorobenzene-d4	6.657

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130321.D
Acq On : 19 Sep 2022 15:19
Operator : CG\JU
Sample : N4656-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

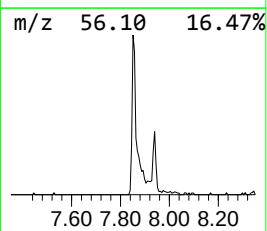
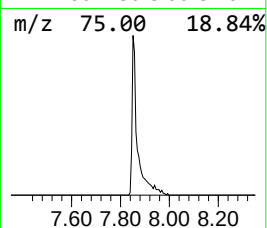
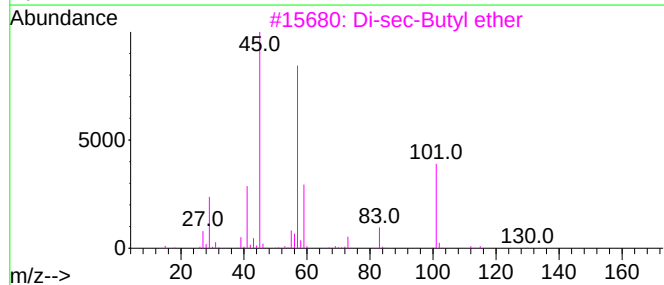
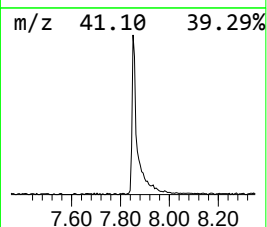
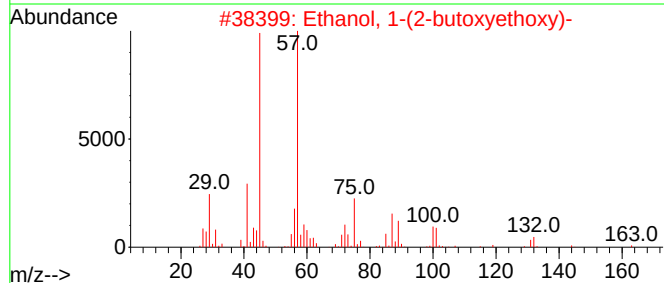
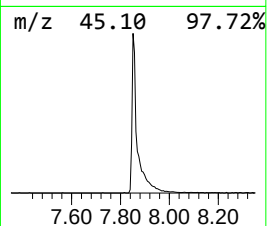
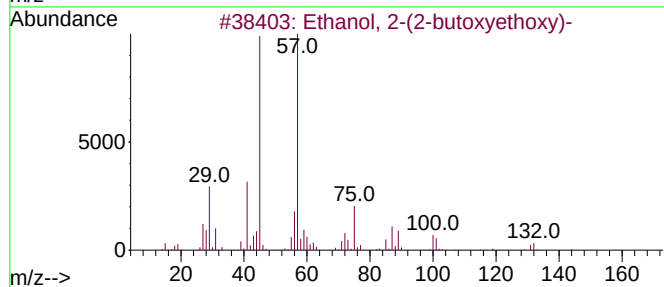
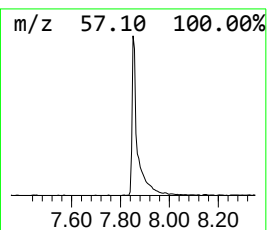
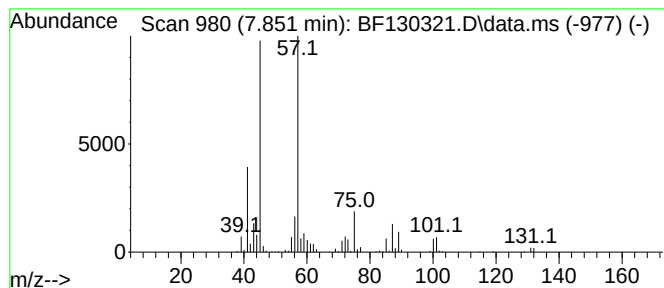
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.851	14.61 ng	545726	Naphthalene-d8	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130321.D
Acq On : 19 Sep 2022 15:19
Operator : CG\JU
Sample : N4656-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

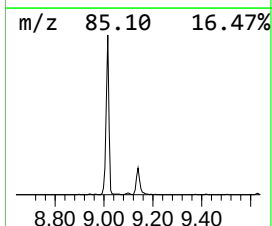
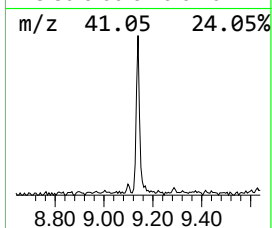
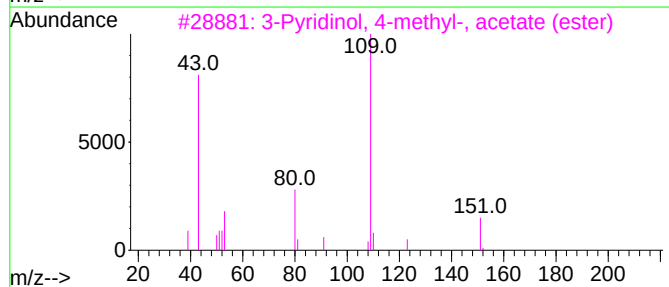
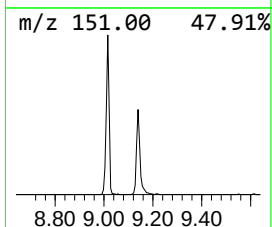
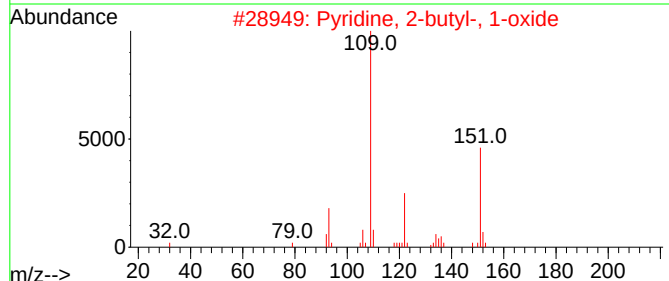
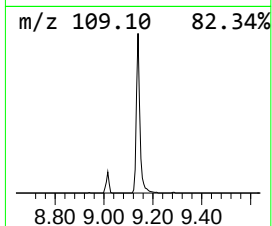
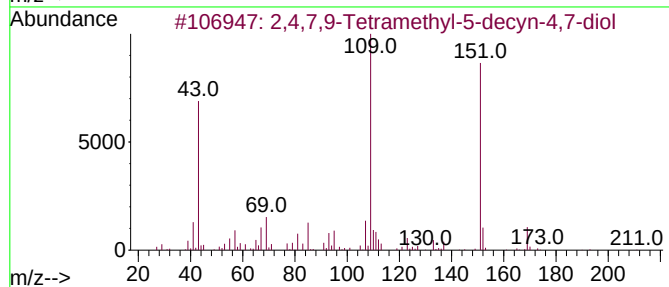
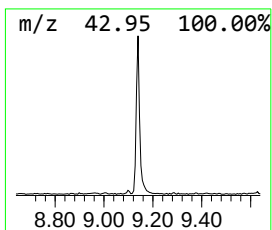
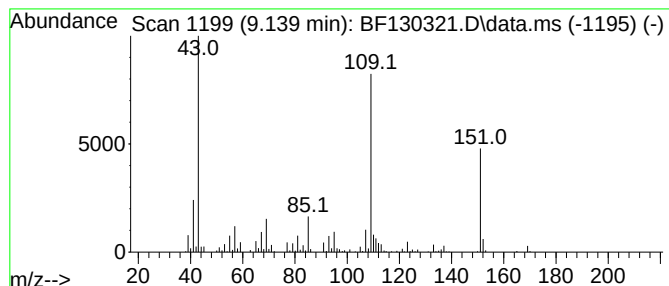
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.139	7.02 ng	285798	Acenaphthene-d10	9.686

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53	
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53	
5	Metacetamol	151	C8H9NO2	000621-42-1	53	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130321.D
Acq On : 19 Sep 2022 15:19
Operator : CG\JU
Sample : N4656-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

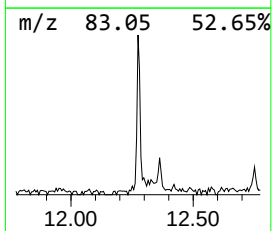
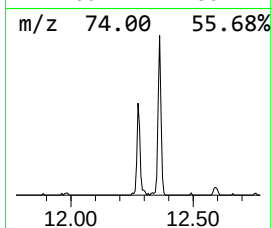
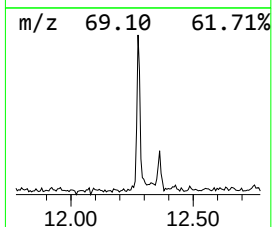
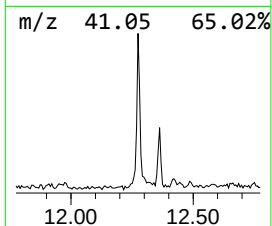
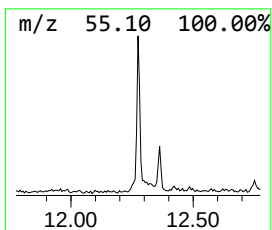
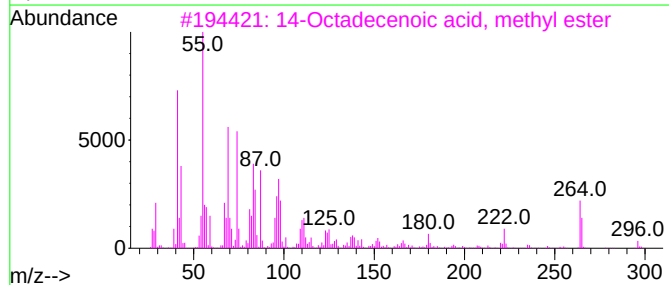
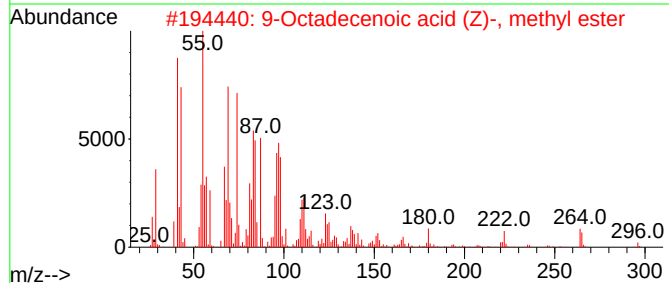
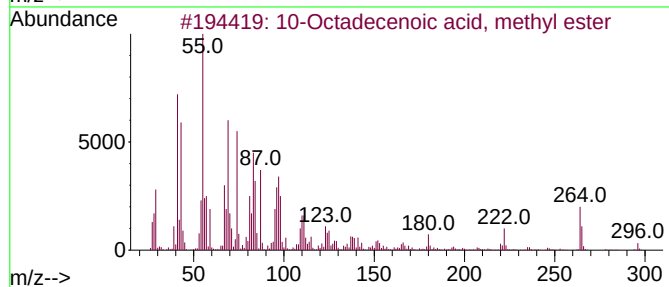
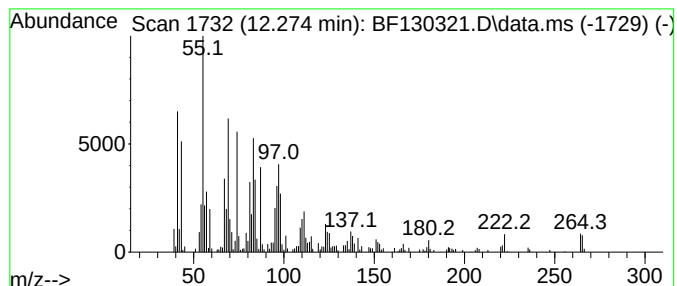
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 10-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.274	5.01 ng	184644	Phenanthrene-d10	11.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
3			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
4			9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	91
5			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130321.D
Acq On : 19 Sep 2022 15:19
Operator : CG\JU
Sample : N4656-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

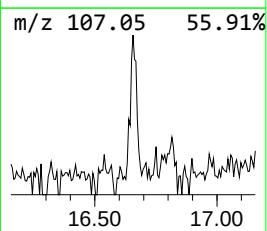
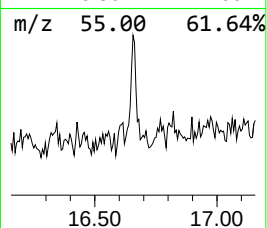
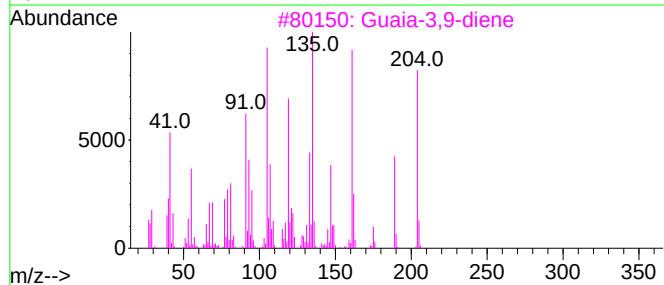
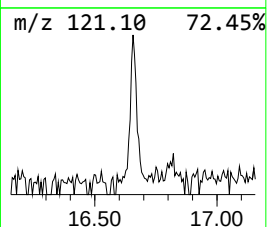
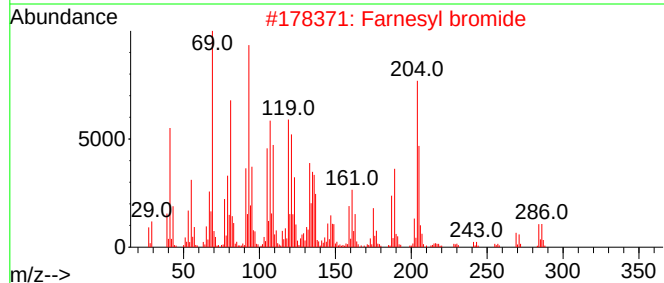
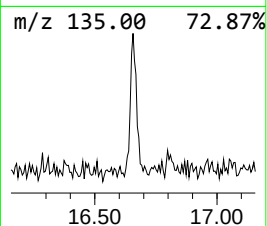
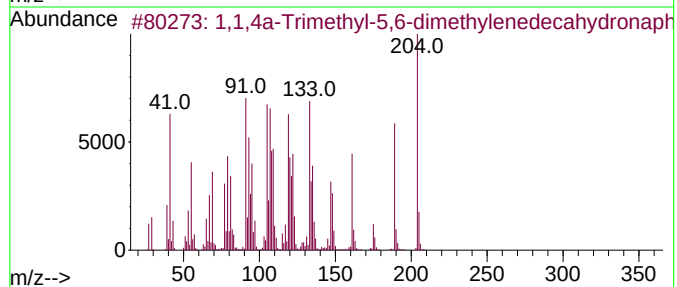
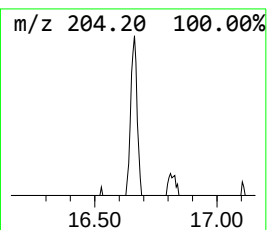
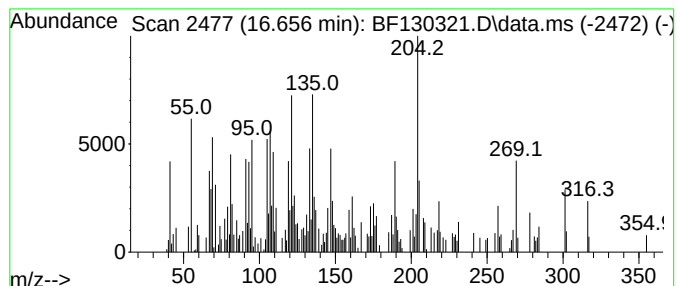
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.657	5.21 ng	129143	Perylene-d12	15.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	62		
2	Farnesyl bromide	284	C15H25Br	006874-67-5	53		
3	Guaia-3,9-diene	204	C15H24	000489-83-8	50		
4	(1R,1aR,2aS,6R,6aS,7aS)-1,6,6a-T...	204	C15H24	026620-70-2	49		
5	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	49		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130321.D
Acq On : 19 Sep 2022 15:19
Operator : CG\JU
Sample : N4656-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

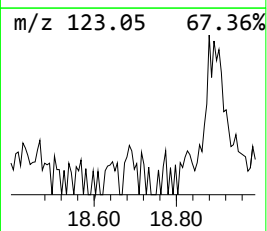
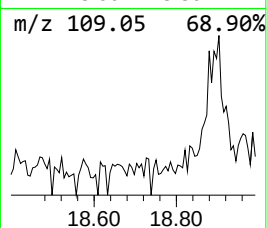
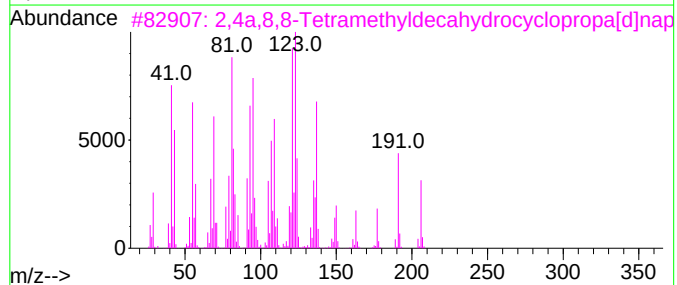
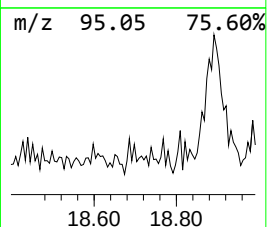
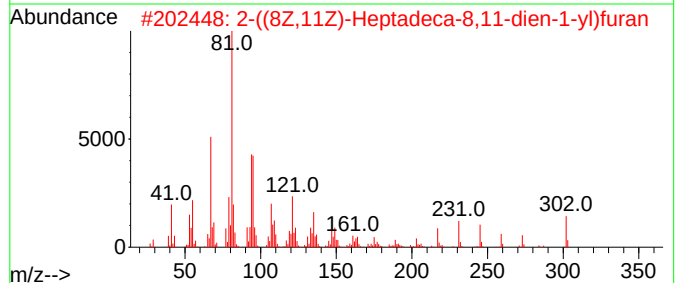
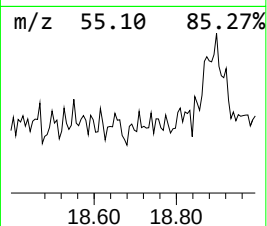
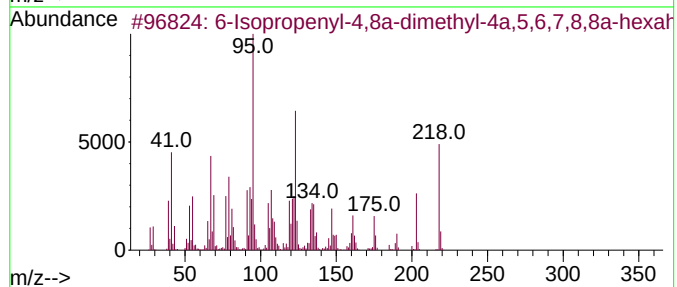
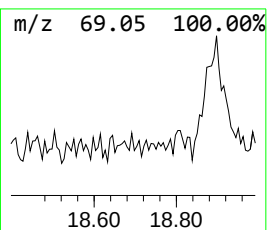
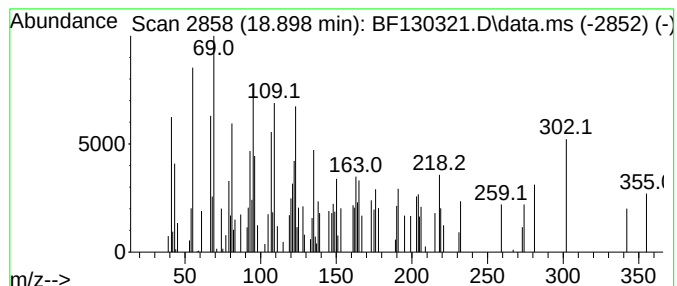
Instrument :
BNA_F
ClientSampleId :
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 6-Isopropenyl-4,8a-dimethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.898	2.47 ng	61254	Perylene-d12	15.186	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	55
2	2-((8Z,11Z)-Heptadeca-8,11-dien-...	302	C21H34O	148675-93-8	45
3	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	45
4	1-((1S,3aR,4S,7R,7aR)-3a,7a-Dime...	206	C14H22O	066748-84-3	38
5	Sesquirosefuran	218	C15H22O	039007-93-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130321.D
Acq On : 19 Sep 2022 15:19
Operator : CG\JU
Sample : N4656-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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-...	4.845	3.9	ng	110334	1	6.657	568805	20.0
Ethanol, 2-(2-b...	7.851	14.6	ng	545726	2	7.939	747188	20.0
2,4,7,9-Tetrame...	9.139	7.0	ng	285798	3	9.686	814765	20.0
10-Octadecenoic...	12.274	5.0	ng	184644	4	11.169	737732	20.0
1,1,4a-Trimethy...	16.657	5.2	ng	129143	6	15.186	495536	20.0
6-Isopropenyl-4...	18.898	2.5	ng	61254	6	15.186	495536	20.0