

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
 Data File : BF135632.D
 Acq On : 06 Oct 2023 16:48
 Operator : CG\JU
 Sample : 04764-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRAVEL

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135632.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.969	487	490	505	rBV	179012	251907	7.72%	1.050%
2	5.375	556	559	588	rBV	2872693	2983054	91.42%	12.434%
3	6.387	728	731	757	rBV	2832429	2998992	91.90%	12.501%
4	6.587	763	765	782	rVB	39476	71667	2.20%	0.299%
5	6.740	787	791	799	rBV	911437	843089	25.84%	3.514%
6	7.304	883	887	900	rBV	2061684	1920082	58.84%	8.004%
7	8.016	1004	1008	1021	rVB	1278867	1141041	34.97%	4.756%
8	9.098	1186	1192	1195	rBV	3339893	3263174	100.00%	13.602%
9	9.216	1208	1212	1227	rVB	371701	383763	11.76%	1.600%
10	9.775	1303	1307	1320	rVB	1499692	1298259	39.79%	5.412%
11	10.569	1438	1442	1456	rBV	1784067	1755743	53.80%	7.319%
12	11.269	1557	1561	1569	rBV	1678595	1404284	43.03%	5.854%
13	11.333	1569	1572	1576	rVB2	34637	37151	1.14%	0.155%
14	11.663	1625	1628	1632	rBV	47042	41624	1.28%	0.174%
15	11.804	1649	1652	1664	rBV3	48244	98613	3.02%	0.411%
16	12.351	1742	1745	1746	rBV	42357	35662	1.09%	0.149%
17	12.375	1746	1749	1752	rVB	175374	147563	4.52%	0.615%
18	12.869	1828	1833	1836	rBV	3265202	3263156	100.00%	13.602%
19	13.439	1926	1930	1933	rBV	49195	44267	1.36%	0.185%
20	13.769	1983	1986	1994	rVB	50462	47504	1.46%	0.198%
21	13.927	2010	2013	2024	rVB	967830	922965	28.28%	3.847%
22	14.086	2037	2040	2043	rBV	43138	40033	1.23%	0.167%
23	14.398	2089	2093	2098	rBV	43499	43343	1.33%	0.181%
24	14.698	2141	2144	2149	rVB	40836	40035	1.23%	0.167%
25	14.769	2152	2156	2161	rVB	79893	82031	2.51%	0.342%
26	15.033	2197	2201	2205	rVB	30613	39540	1.21%	0.165%
27	15.398	2258	2263	2273	rBV	563128	791603	24.26%	3.300%

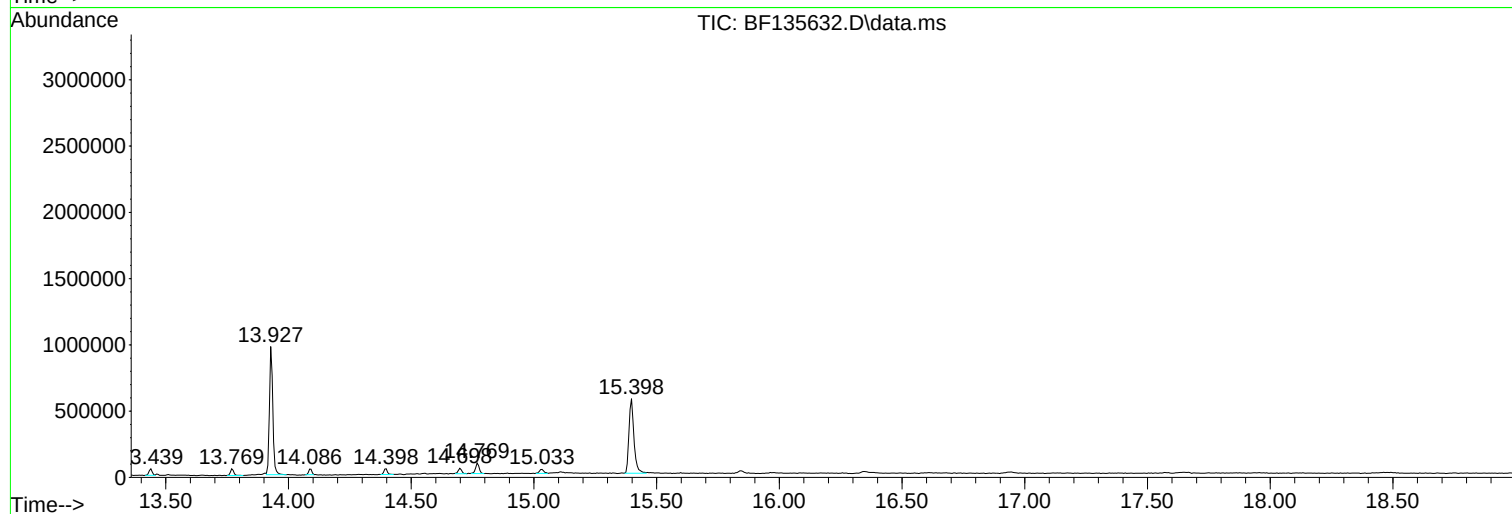
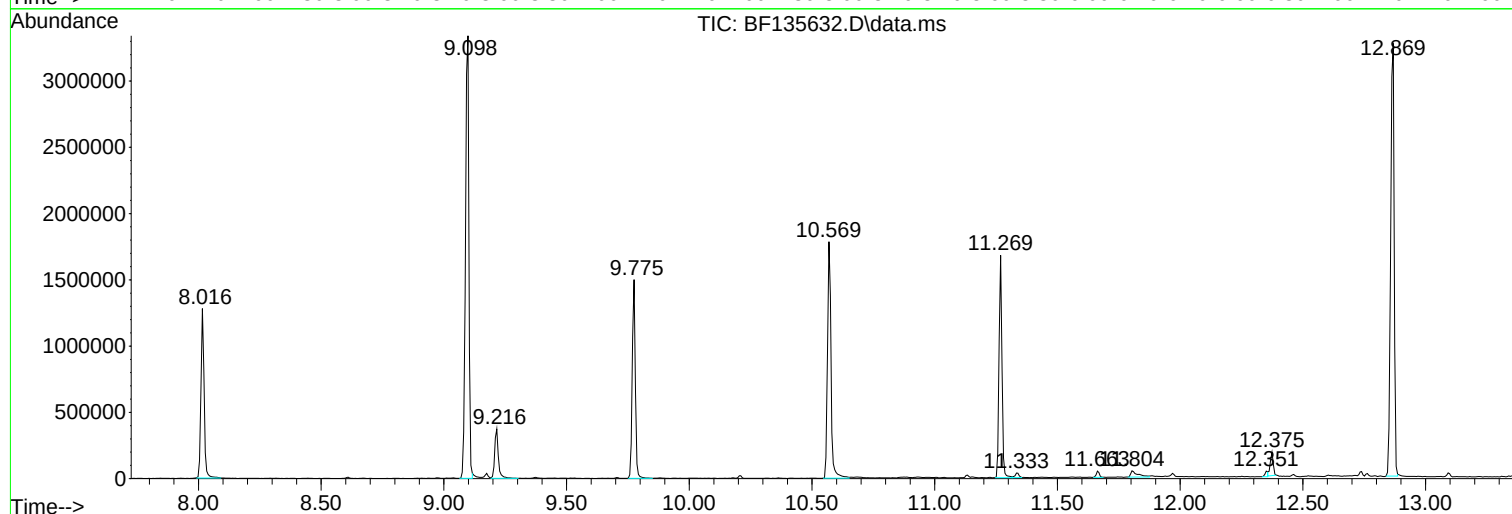
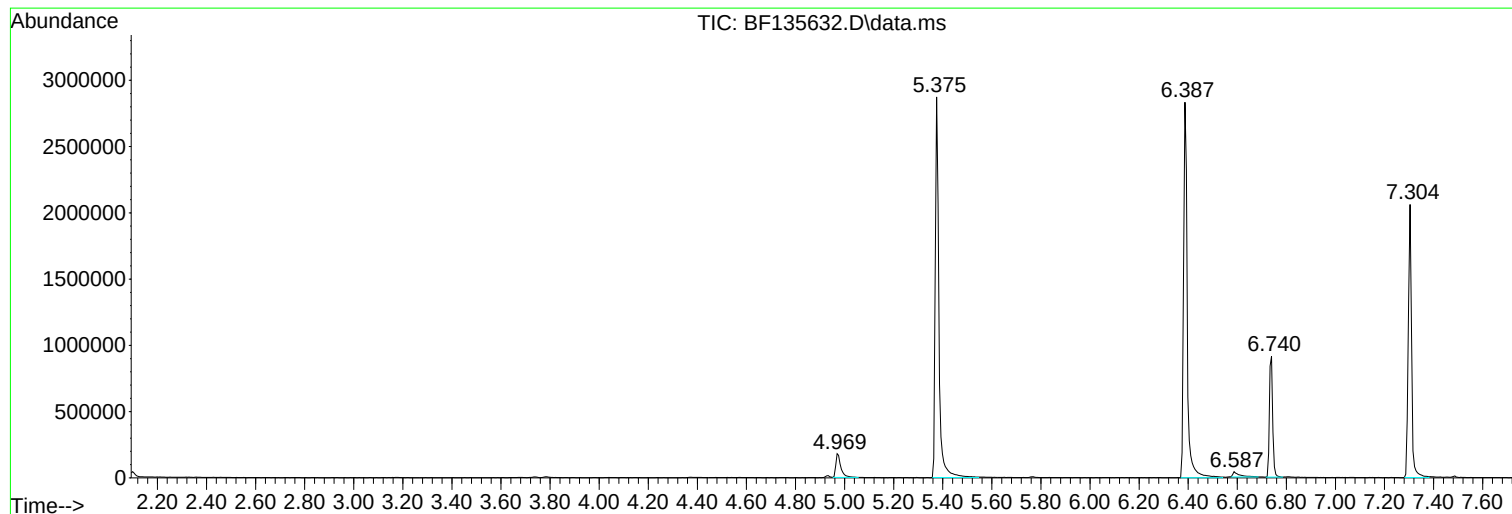
Sum of corrected areas: 23990145

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
Data File : BF135632.D
Acq On : 06 Oct 2023 16:48
Operator : CG\JU
Sample : 04764-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRAVEL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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\BF100623\
Data File : BF135632.D
Acq On : 06 Oct 2023 16:48
Operator : CG\JU
Sample : 04764-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

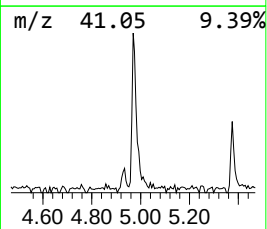
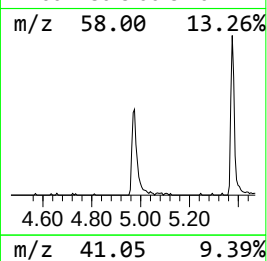
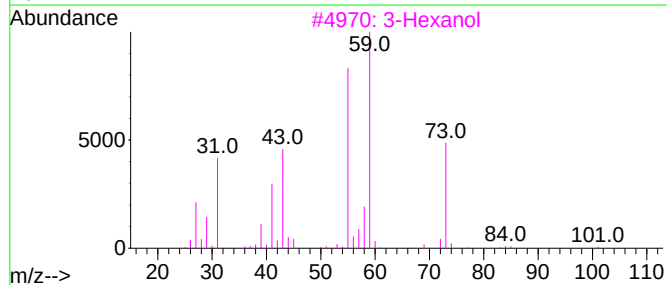
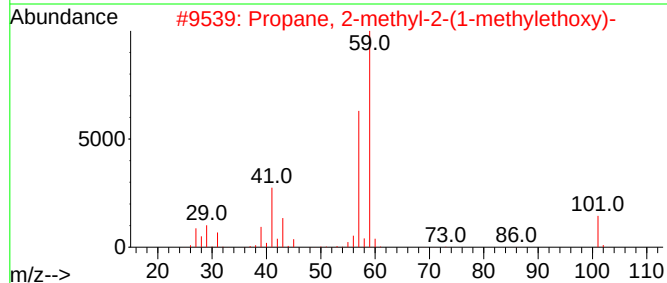
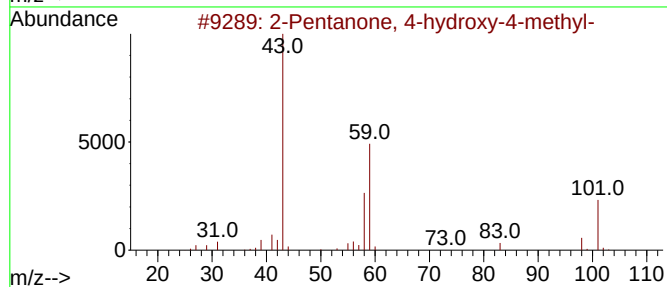
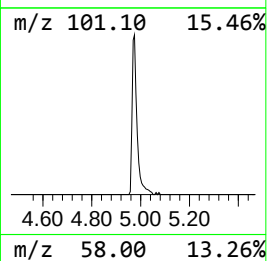
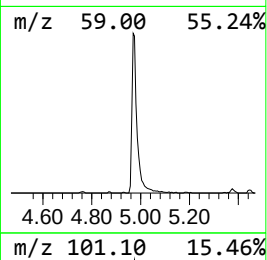
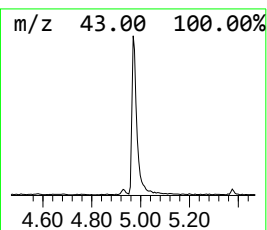
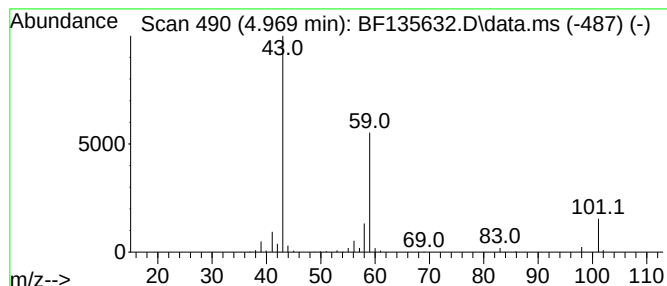
Instrument :
BNA_F
ClientSampleId :
GRAVEL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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.
4.969	5.98 ng	251907	1,4-Dichlorobenzene-d4			6.740
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	36
3	3-Hexanol		102	C6H14O	000623-37-0	33
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	32
5	Butyl aldoxime, 3-methyl-, syn-		101	C5H11NO	005780-40-5	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
Data File : BF135632.D
Acq On : 06 Oct 2023 16:48
Operator : CG\JU
Sample : 04764-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRAVEL

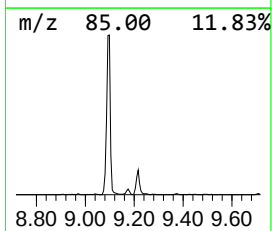
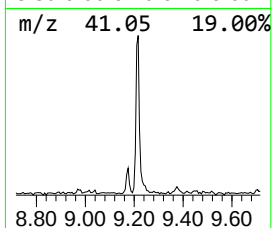
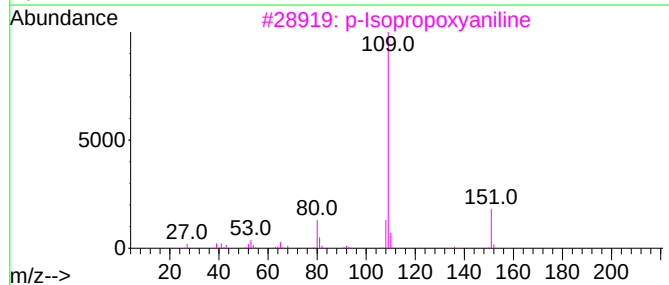
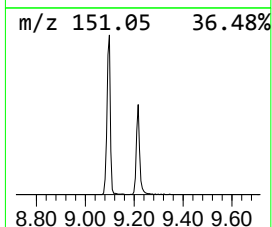
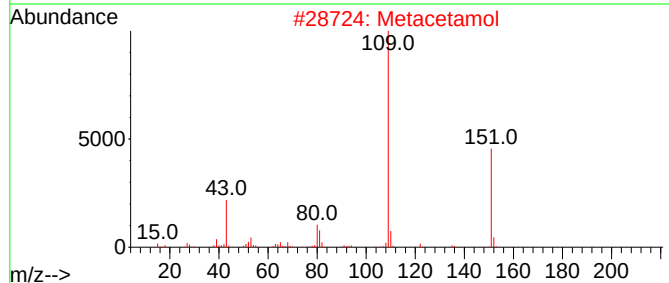
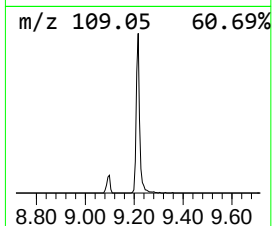
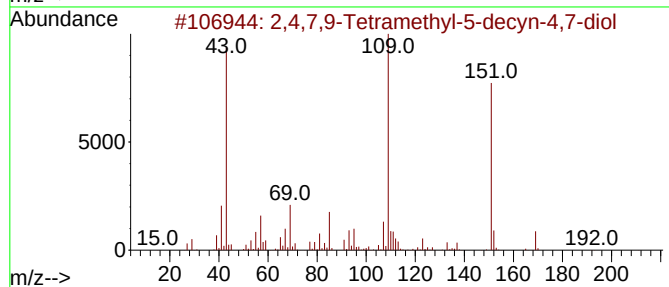
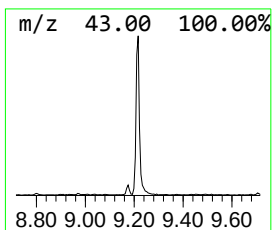
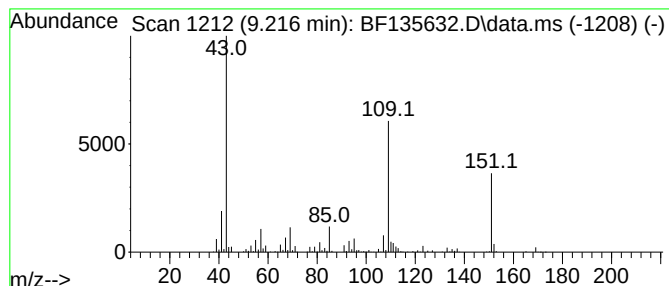
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	5.91 ng	383763	Acenaphthene-d10	9.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87	
2	Metacetamol	151	C8H9NO2	000621-42-1	47	
3	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	47	
4	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	47	
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	47	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
Data File : BF135632.D
Acq On : 06 Oct 2023 16:48
Operator : CG\JU
Sample : 04764-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRAVEL

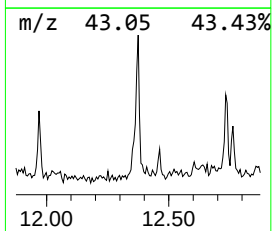
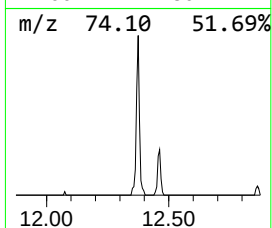
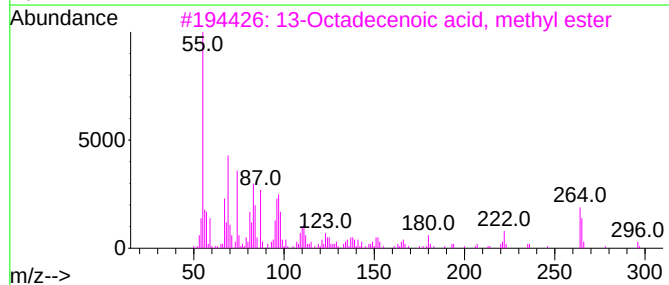
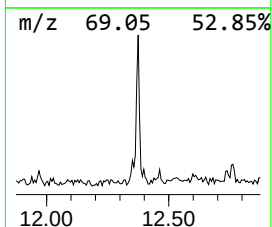
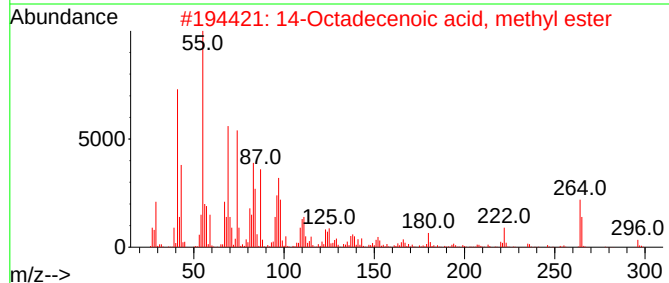
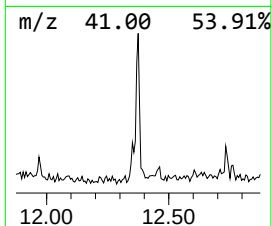
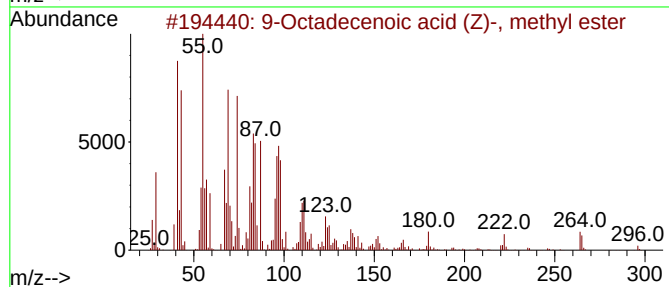
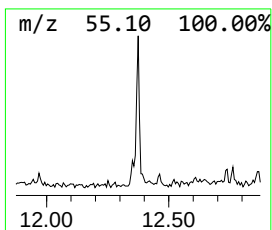
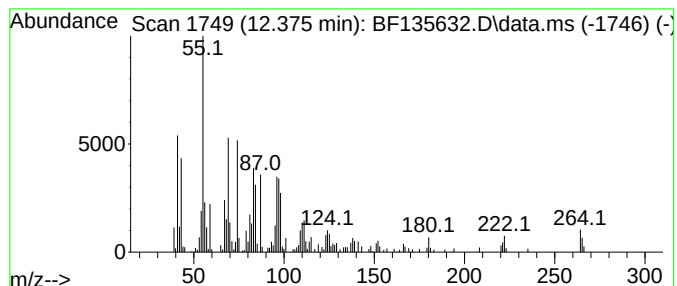
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.375	2.10 ng	147563	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
2			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
3			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
4			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	90
5			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
Data File : BF135632.D
Acq On : 06 Oct 2023 16:48
Operator : CG\JU
Sample : 04764-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRAVEL

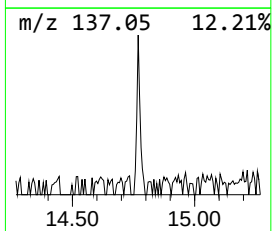
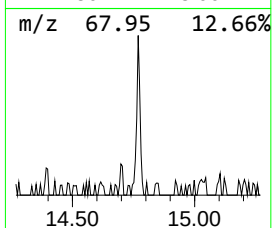
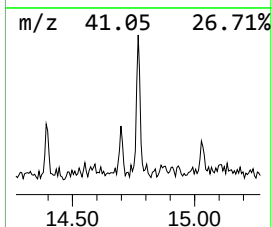
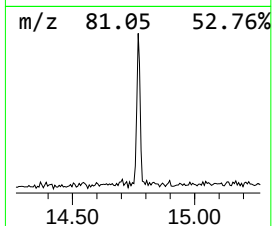
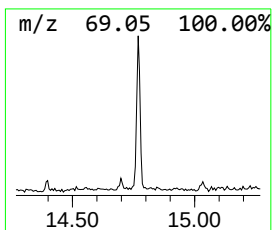
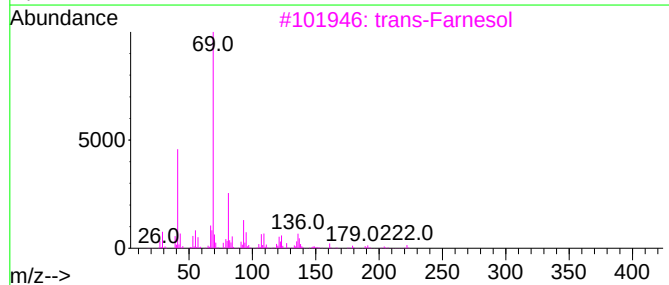
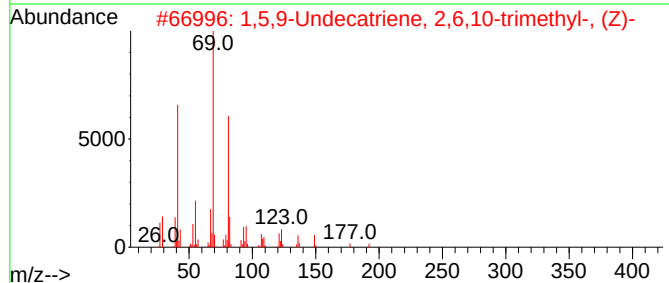
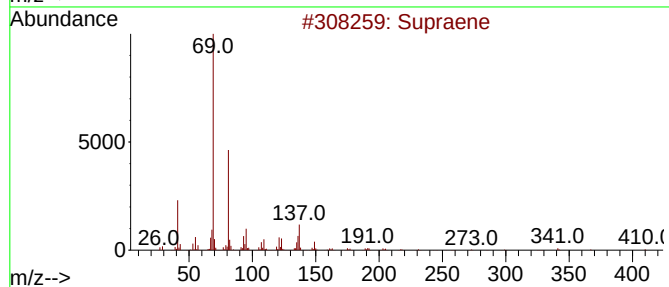
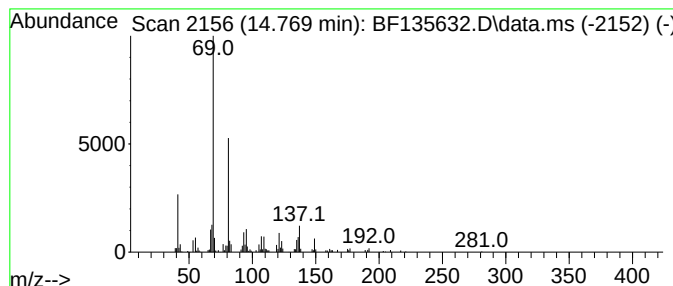
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.769	2.07 ng	82031	Perylene-d12	15.398

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	80
3			trans-Farnesol	222	C15H26O	000106-28-5	72
4			Propanoic acid, 2,2-dimethyl-, [...]	306	C20H34O2	1000164-38-8	72
5			Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100623\
Data File : BF135632.D
Acq On : 06 Oct 2023 16:48
Operator : CG\JU
Sample : 04764-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRAVEL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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-...	4.969	6.0	ng	251907	1	6.740	843089	20.0
2,4,7,9-Tetrame...	9.216	5.9	ng	383763	3	9.775	1298260	20.0
9-Octadecenoic ...	12.375	2.1	ng	147563	4	11.269	1404280	20.0
Supraene	14.769	2.1	ng	82031	6	15.398	791603	20.0