

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
 Data File : BF123644.D
 Acq On : 20 Apr 2021 15:44
 Operator : JU/CG
 Sample : M2081-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EFF-WW

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-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123644.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.416	211	226	230	rBV	5006649	10954572	2.39%	0.964%
2	4.163	343	353	356	rBV	4090084	6650807	1.45%	0.586%
3	5.475	572	576	586	rVB	5786275	5554447	1.21%	0.489%
4	6.981	817	832	834	rBV	28577676	93064829	20.30%	8.193%
5	7.010	834	837	848	rVB	7253474	8005040	1.75%	0.705%
6	7.422	900	907	910	rVB	7164983	7790912	1.70%	0.686%
7	7.616	921	940	941	rBV2	1994299	6534480	1.43%	0.575%
8	8.139	988	1029	1031	rBV	12087539	72544149	15.82%	6.387%
9	8.198	1036	1039	1040	rVV2	17204476	20439647	4.46%	1.800%
10	8.216	1040	1042	1045	rVB	16386541	12460856	2.72%	1.097%
11	9.016	1173	1178	1181	rBV	5249845	4875820	1.06%	0.429%
12	9.122	1182	1196	1198	rBV	9555855	18486142	4.03%	1.628%
13	9.222	1209	1213	1215	rBV	10426631	10534207	2.30%	0.927%
14	9.710	1293	1296	1308	rBV	3734701	4847675	1.06%	0.427%
15	9.898	1319	1328	1331	rBV	6089118	5558328	1.21%	0.489%
16	10.110	1360	1364	1366	rVV	6846335	7744418	1.69%	0.682%
17	10.463	1366	1424	1427	rVB2	37586128	458538590	100.00%	40.370%
18	10.698	1458	1464	1467	rBV2	6874012	7234391	1.58%	0.637%
19	11.221	1527	1553	1555	rBV	28421498	139713447	30.47%	12.300%
20	12.010	1669	1687	1699	rVV2	22402027	85541342	18.66%	7.531%
21	12.721	1786	1808	1812	rBV2	27214361	106260331	23.17%	9.355%
22	12.774	1812	1817	1824	rVV	17208954	22751667	4.96%	2.003%
23	12.933	1841	1844	1847	rVV	5864989	4836291	1.05%	0.426%
24	12.992	1849	1854	1857	rVB	9922896	10186821	2.22%	0.897%
25	15.198	2225	2229	2240	rVB	2956140	4732126	1.03%	0.417%

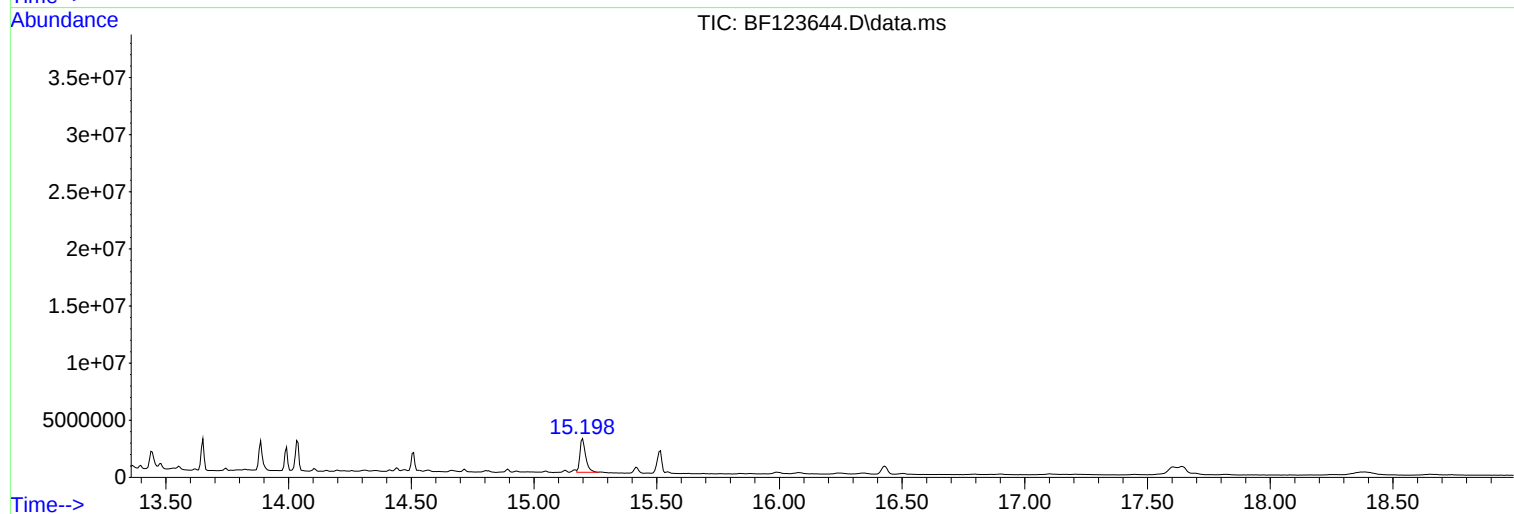
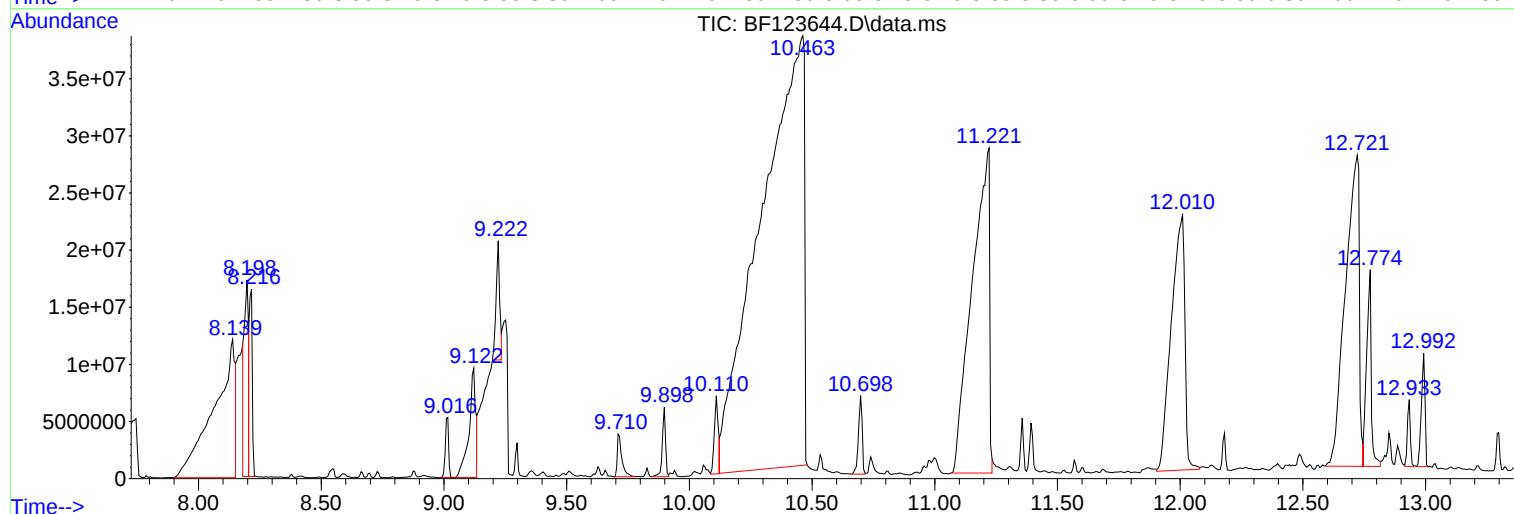
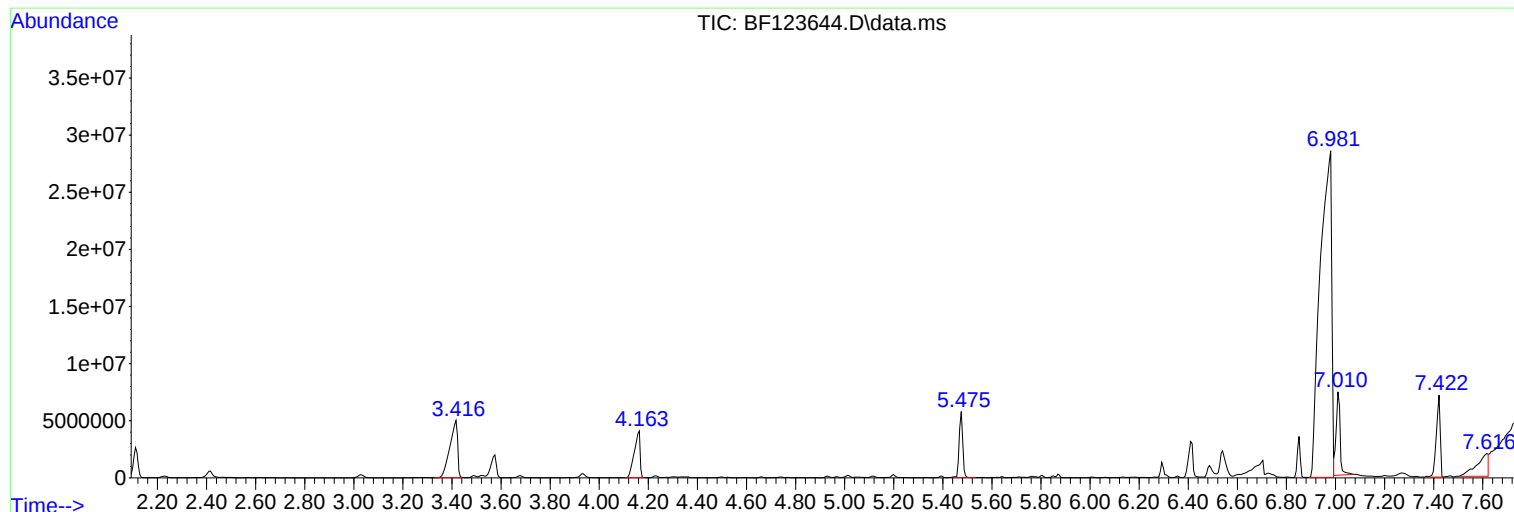
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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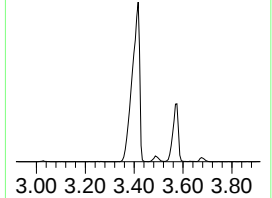
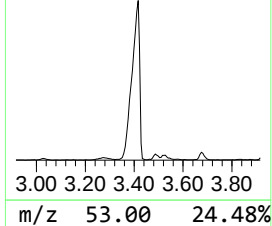
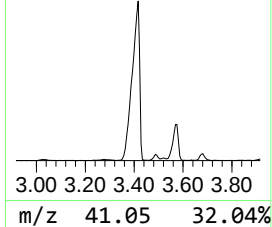
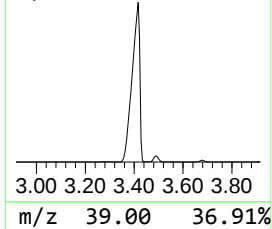
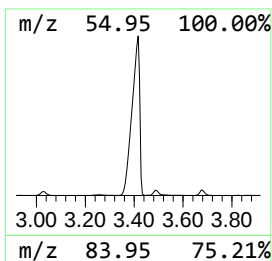
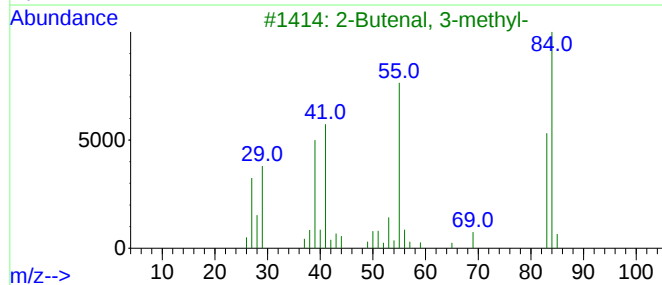
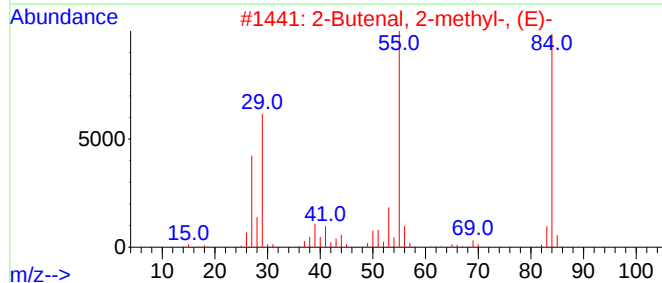
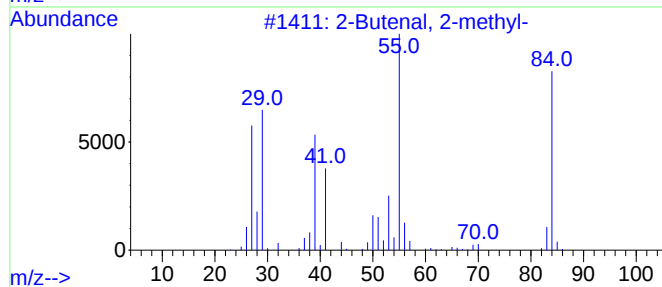
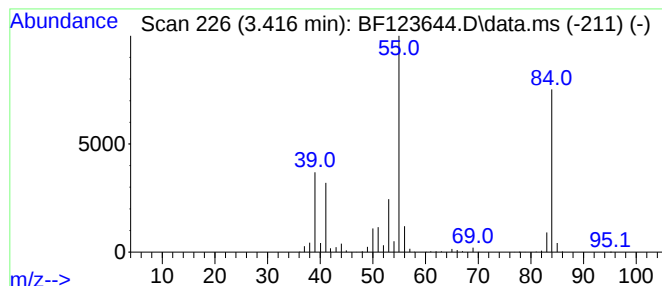
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Butenal, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.416	2.35 ng	10954600	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 2-methyl-			84	C5H8O	001115-11-3	91
2	2-Butenal, 2-methyl-, (E)-			84	C5H8O	000497-03-0	90
3	2-Butenal, 3-methyl-			84	C5H8O	000107-86-8	87
4	2-Ethylacrolein			84	C5H8O	000922-63-4	80
5	2-Pentenal, (E)-			84	C5H8O	001576-87-0	64



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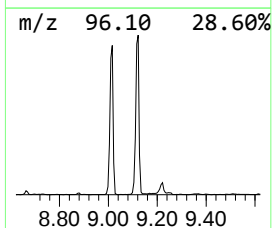
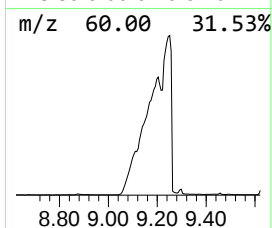
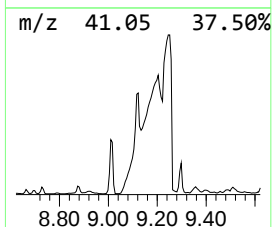
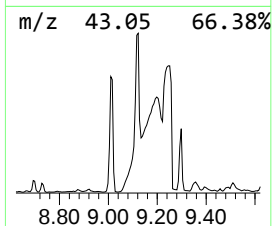
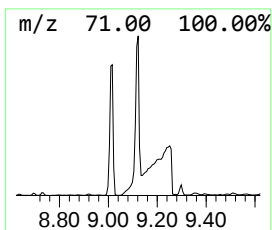
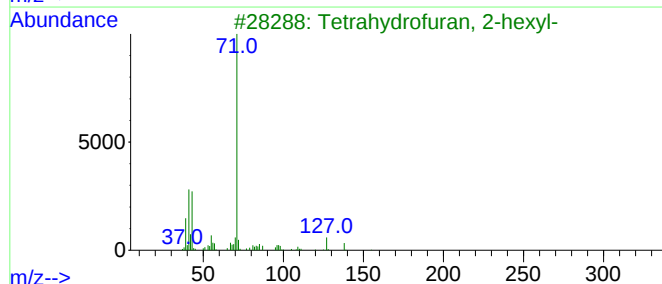
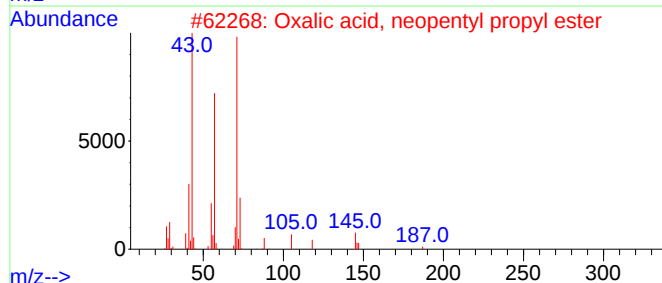
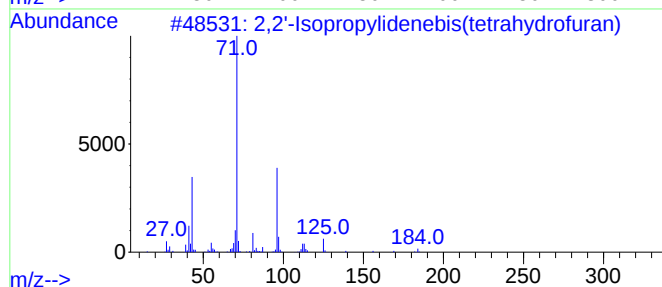
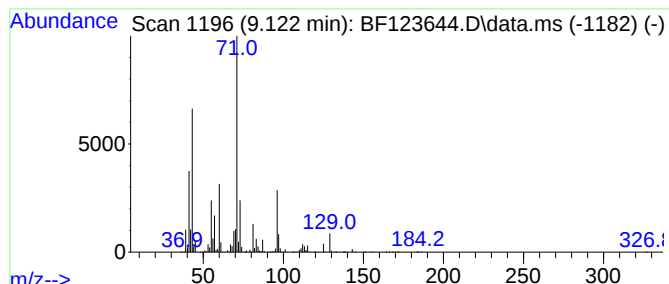
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Peak Number 2 2,2'-Isopropylidenebis(tetr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.122	66.52 ng	18486100	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2'-Isopropylidenebis(tetrahydr...	184	C11H20O2	089686-69-1	58
2			Oxalic acid, neopentyl propyl ester	202	C10H18O4	1000309-72-5	43
3			Tetrahydrofuran, 2-hexyl-	156	C10H20O	003208-32-0	38
4			Hexanoic acid, 3-oxo-, ethyl ester	158	C8H14O3	003249-68-1	38
5			2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	35



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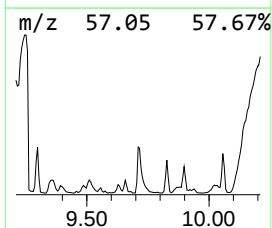
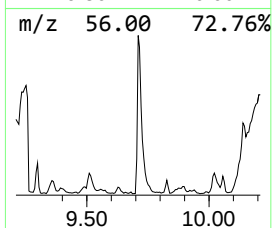
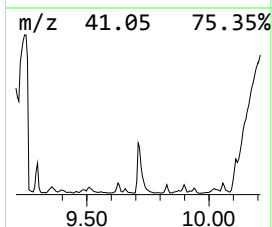
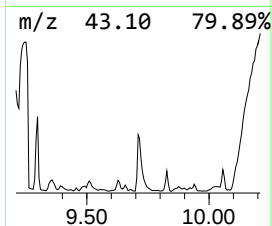
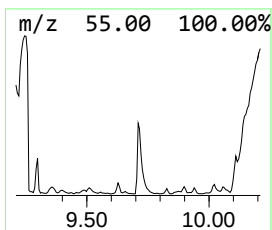
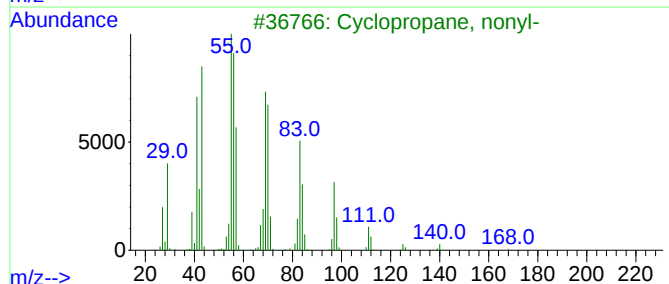
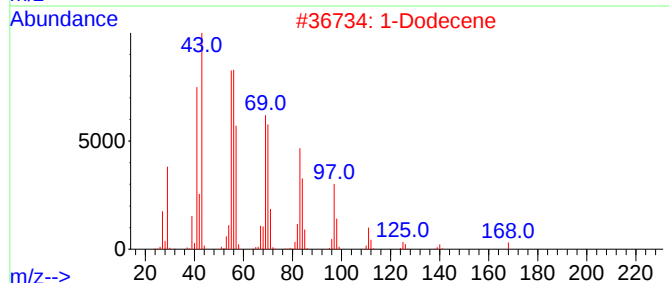
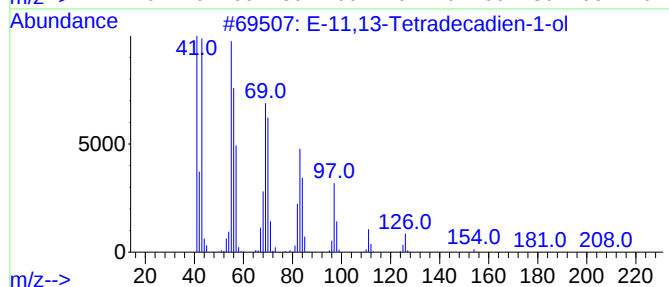
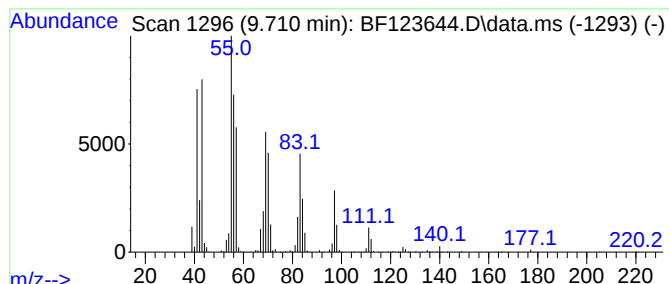
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 E-11,13-Tetradecadien-1-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.710	17.44 ng	4847680	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-11,13-Tetradecadien-1-ol	210	C14H26O	1000131-00-3	91		
2	1-Dodecene	168	C12H24	000112-41-4	91		
3	Cyclopropane, nonyl-	168	C12H24	074663-85-7	91		
4	4-Dodecene, (Z)-	168	C12H24	007206-27-1	90		
5	2-Tetradecene, (E)-	196	C14H28	035953-54-9	90		



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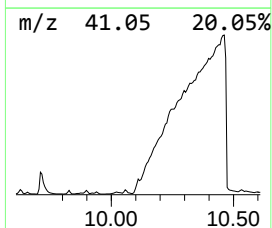
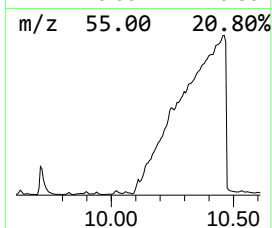
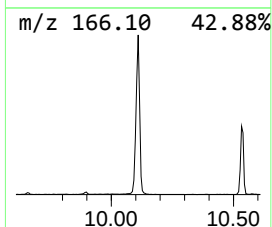
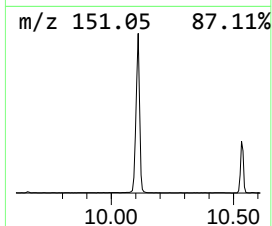
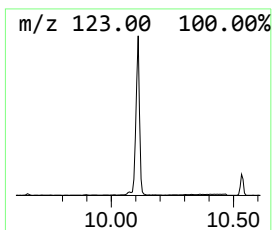
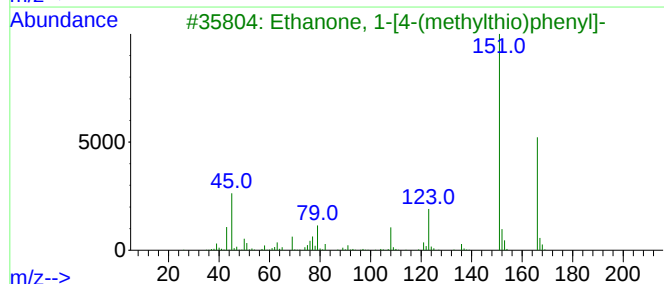
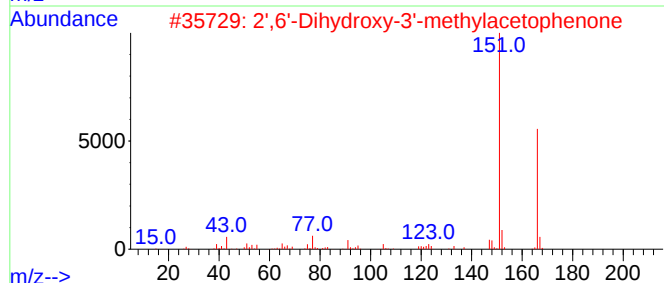
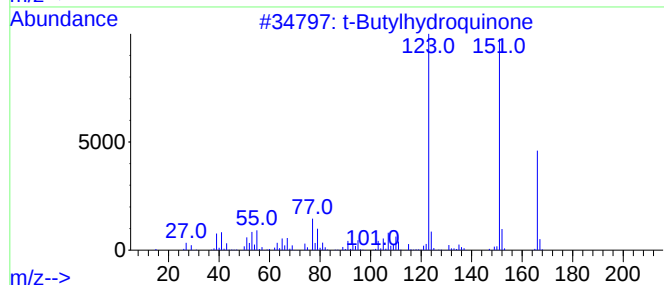
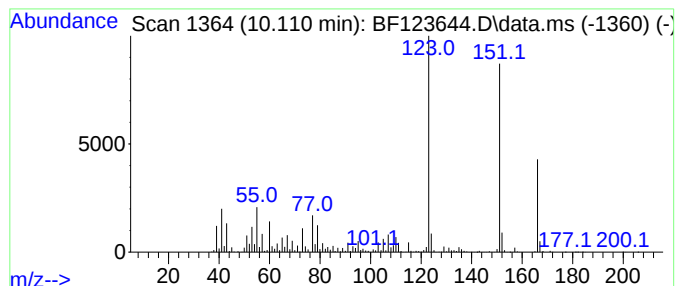
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Peak Number 4 t-Butylhydroquinone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.110	27.87 ng	7744420	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			t-Butylhydroquinone	166	C10H14O2	001948-33-0	96
2			2',6'-Dihydroxy-3'-methylacetoph...	166	C9H10O3	029183-78-6	46
3			Ethanone, 1-[4-(methylthio)phenyl]-	166	C9H10OS	001778-09-2	46
4			Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	46
5			Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	46



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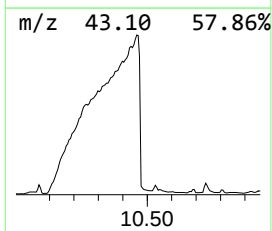
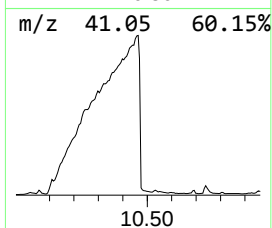
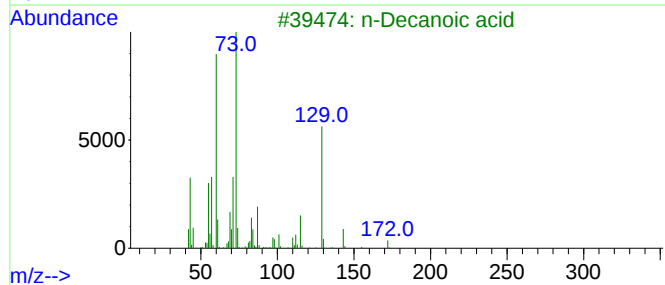
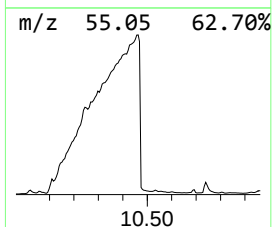
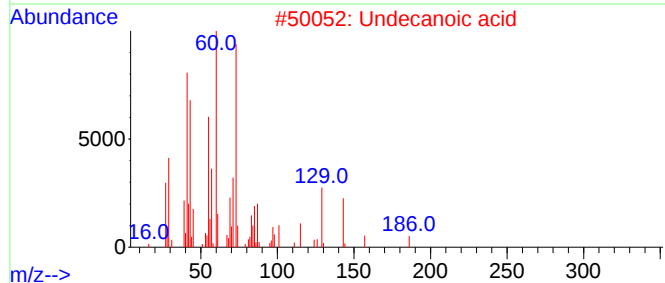
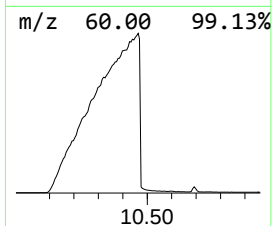
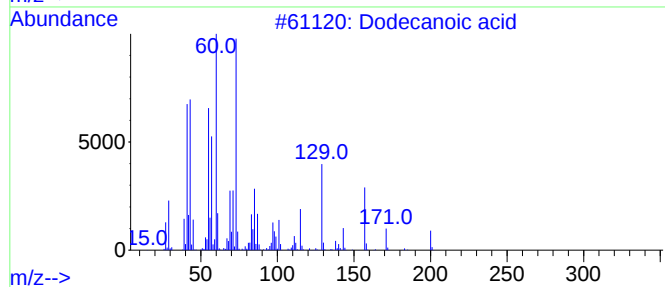
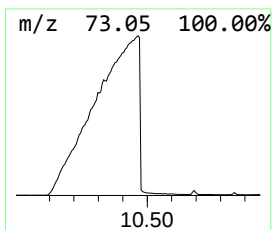
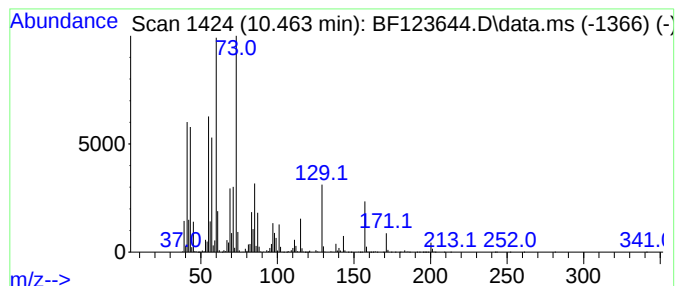
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.463	1649.92 ng	458539000	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	98
2			Undecanoic acid	186	C11H22O2	000112-37-8	72
3			n-Decanoic acid	172	C10H20O2	000334-48-5	68
4			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	43
5			Butanoic acid	88	C4H8O2	000107-92-6	35



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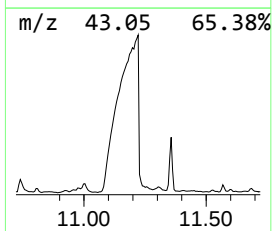
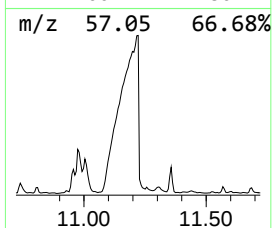
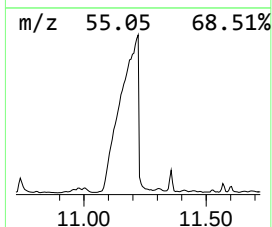
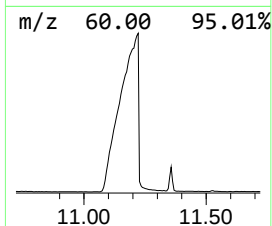
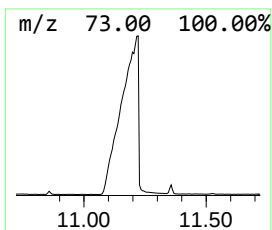
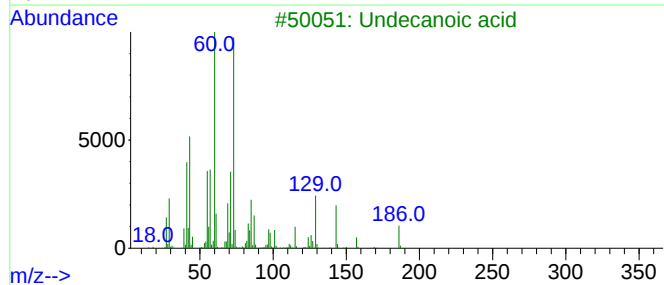
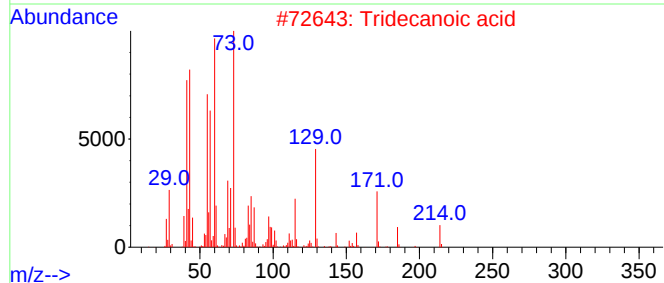
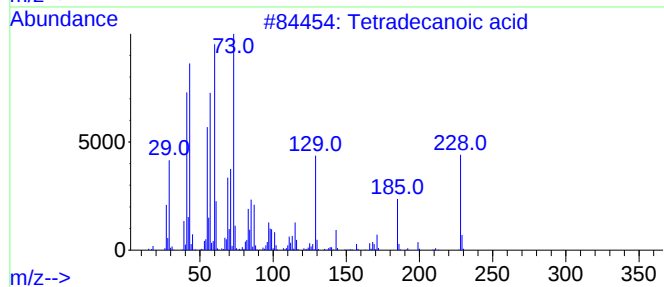
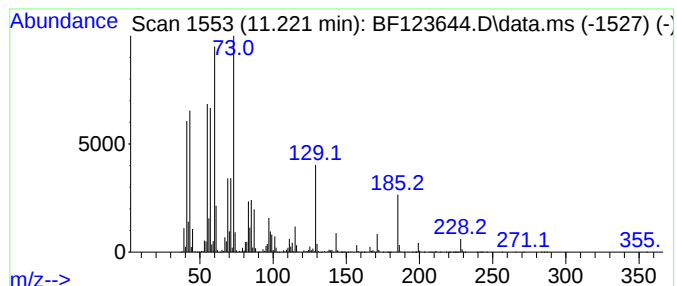
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.221	20.00 ng	139713000	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	87
3			Undecanoic acid	186	C11H22O2	000112-37-8	76
4			Dodecanoic acid	200	C12H24O2	000143-07-7	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123644.D
Acq On : 20 Apr 2021 15:44
Operator : JU/CG
Sample : M2081-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EFF-WW

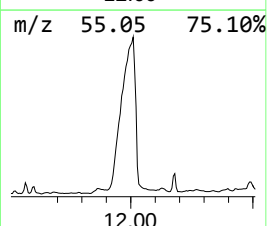
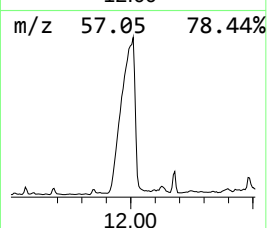
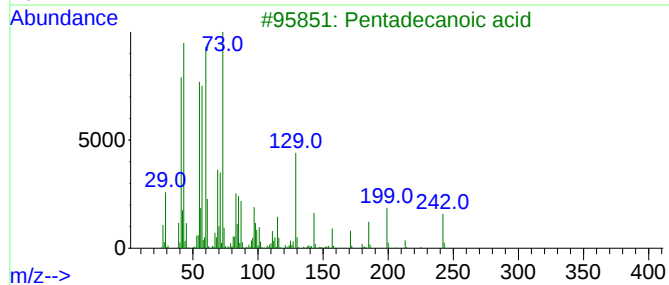
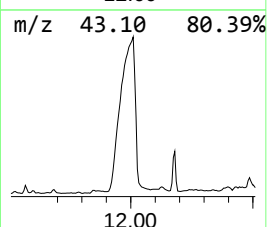
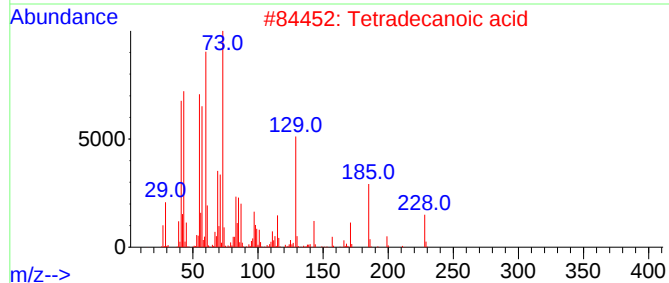
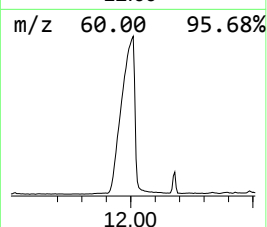
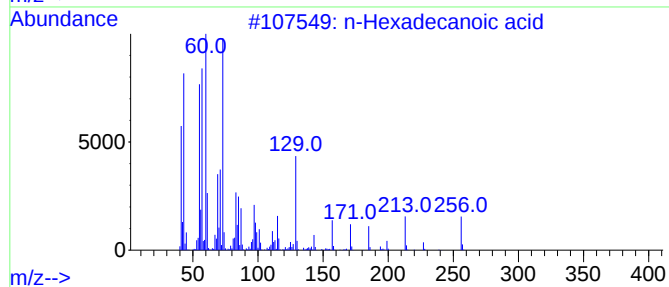
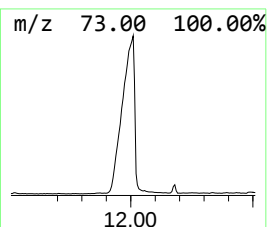
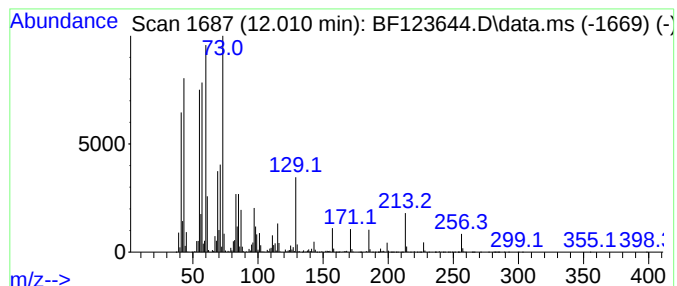
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	12.25 ng	85541300	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	87
5			Estra-1,3,5(10)-trien-17.β-ol	256	C18H24O	002529-64-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123644.D
Acq On : 20 Apr 2021 15:44
Operator : JU/CG
Sample : M2081-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EFF-WW

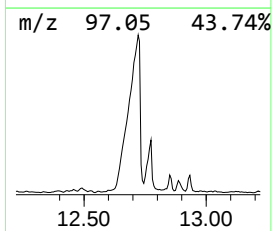
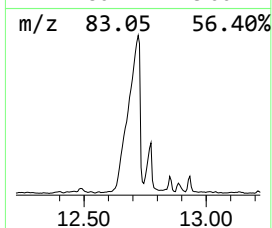
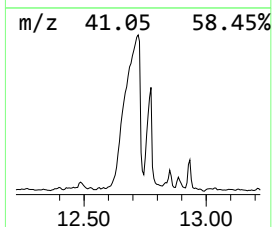
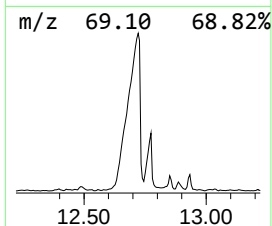
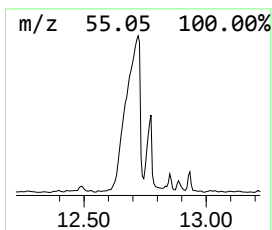
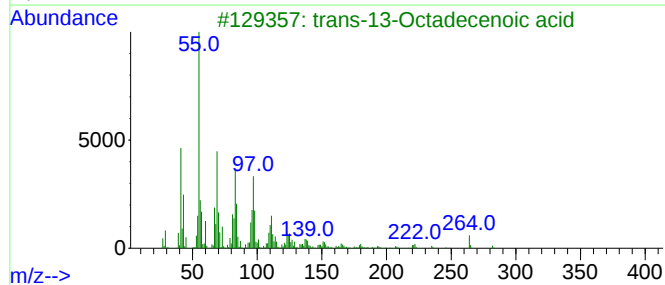
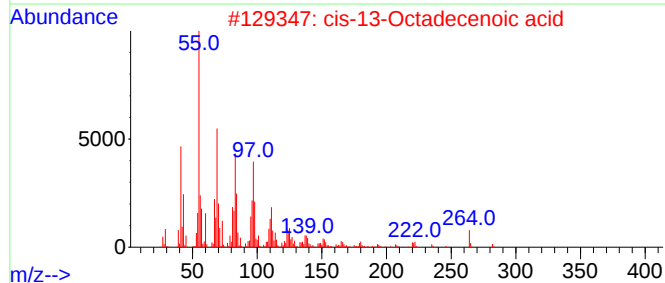
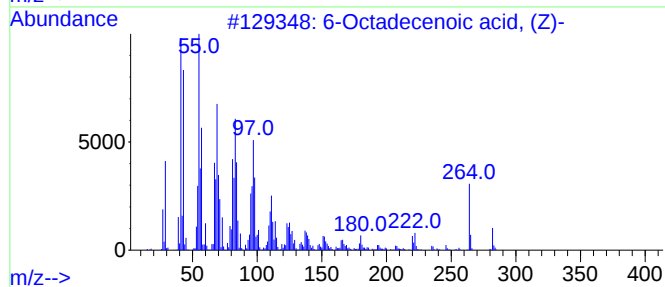
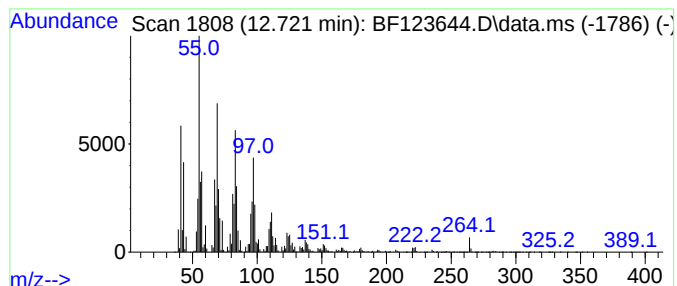
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 6-Octadecenoic acid, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.721	208.62 ng	106260000	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	98
2			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	97
3			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	97
4			6-Octadecenoic acid	282	C18H34O2	1000336-66-8	96
5			Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123644.D
Acq On : 20 Apr 2021 15:44
Operator : JU/CG
Sample : M2081-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EFF-WW

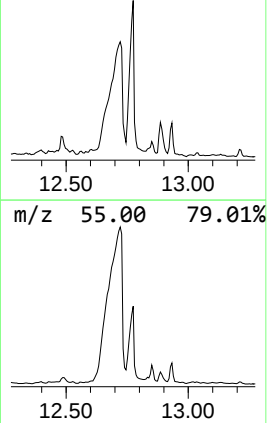
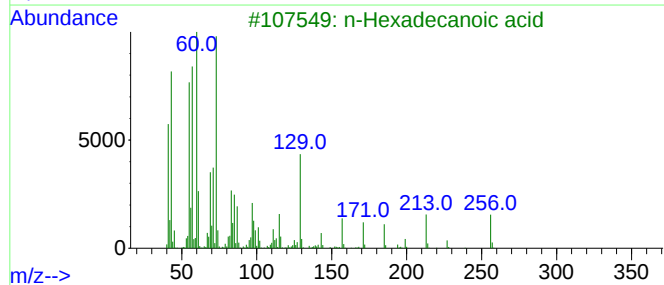
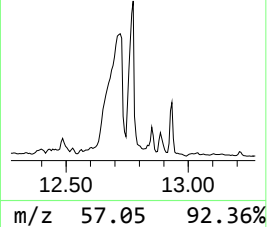
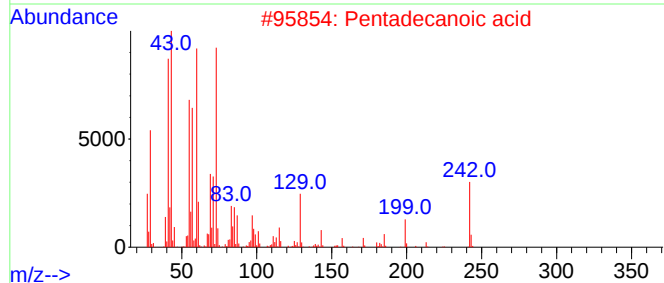
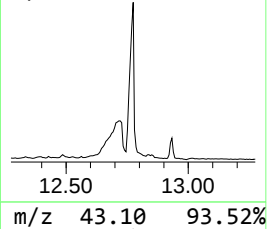
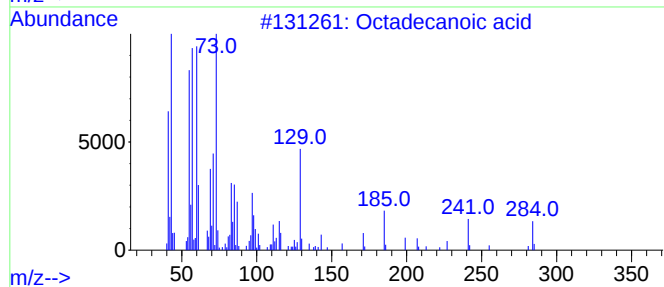
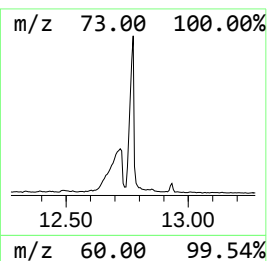
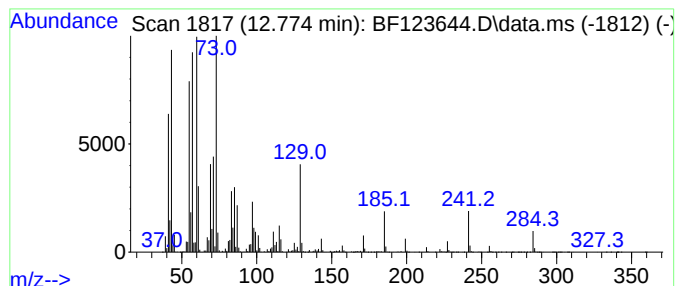
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.774	44.67 ng	22751700	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123644.D
Acq On : 20 Apr 2021 15:44
Operator : JU/CG
Sample : M2081-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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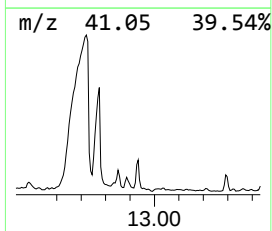
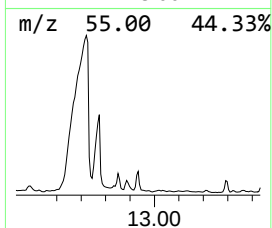
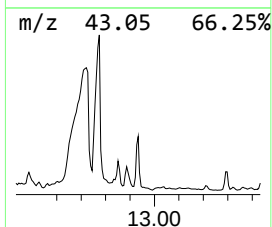
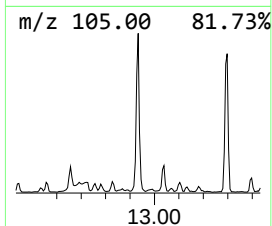
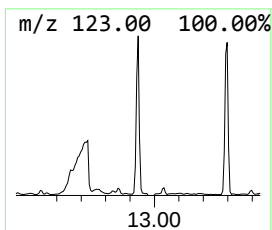
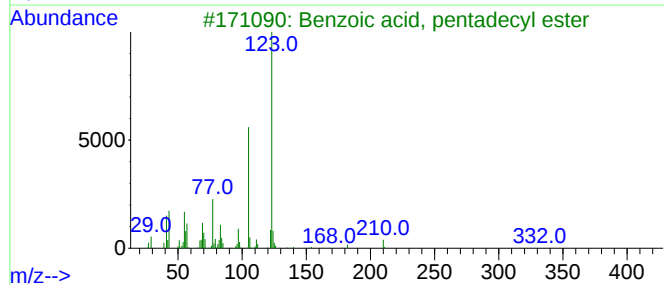
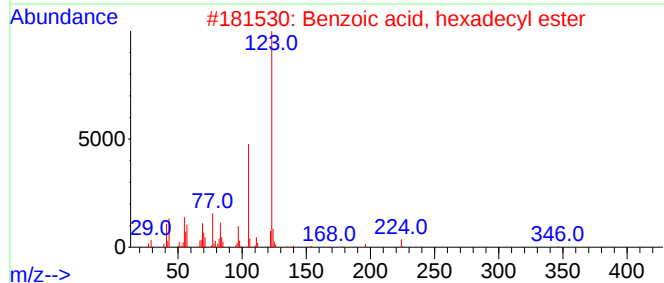
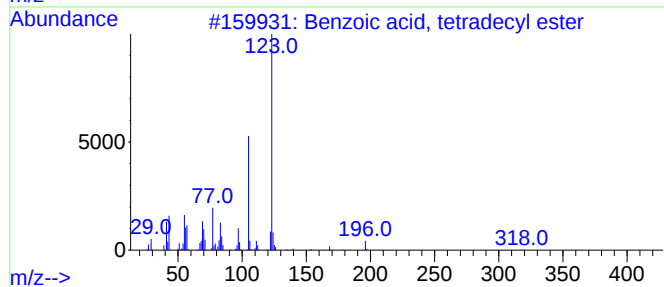
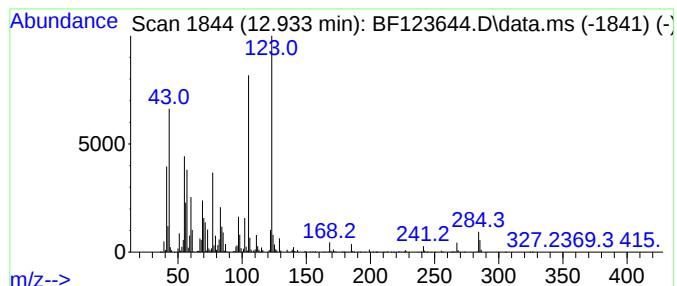
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzoic acid, tetradecyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.933	9.50 ng	4836290	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	76
2			Benzoic acid, hexadecyl ester	346	C23H38O2	1000340-22-9	72
3			Benzoic acid, pentadecyl ester	332	C22H36O2	1000340-22-8	59
4			Benzoic acid, tridecyl ester	304	C20H32O2	1000340-22-6	58
5			Benzoic acid, octadecyl ester	374	C25H42O2	1000340-23-1	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123644.D
Acq On : 20 Apr 2021 15:44
Operator : JU/CG
Sample : M2081-01
Misc :
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Instrument :
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ClientSampleId :
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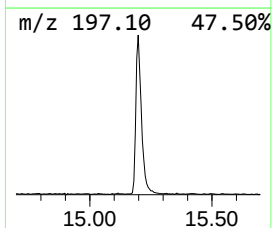
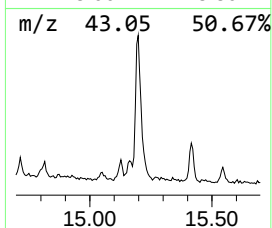
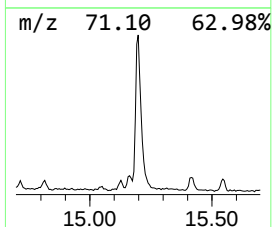
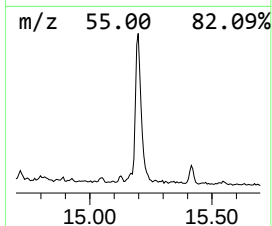
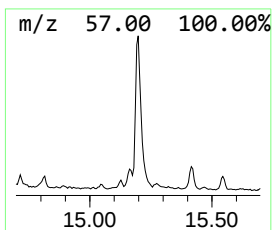
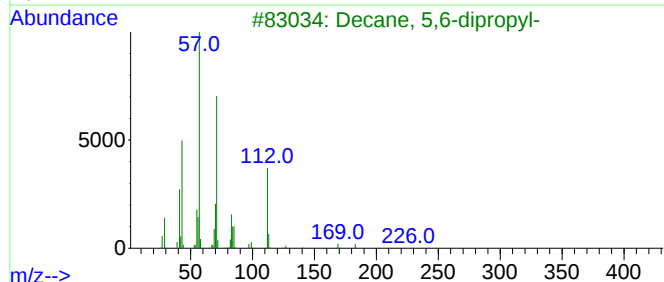
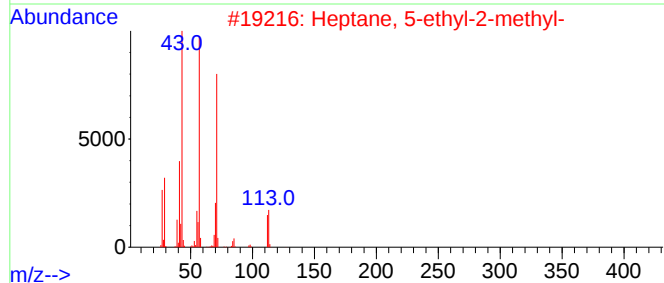
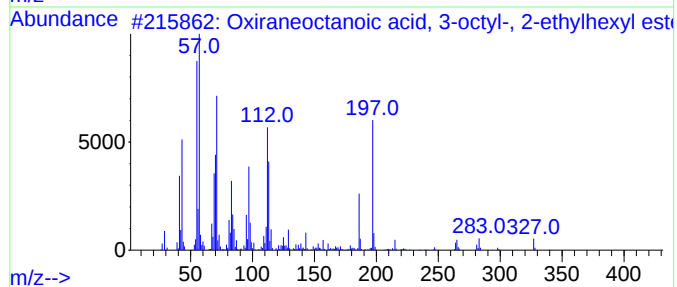
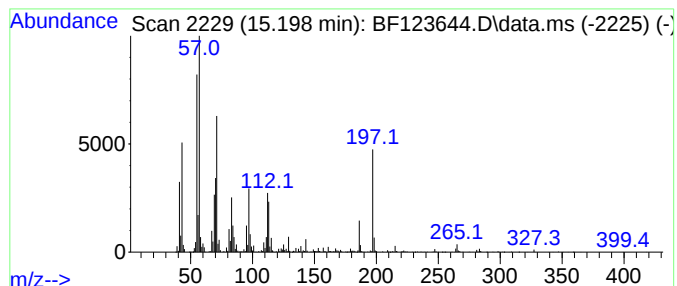
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Oxiraneoctanoic acid, 3-oct... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	20.00 ng	4732130	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxiraneoctanoic acid, 3-octyl-, ...	410	C26H50O3	000141-38-8	58
2			Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	27
3			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	27
4			Methoxyacetic acid, 2-ethylhexyl...	202	C11H22O3	1000282-41-4	27
5			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
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Sample : M2081-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2,2'-Isopropyl...	9.122	66.5	ng	18486100	3	9.898	5558330	20.0
E-11,13-Tetrad...	9.710	17.4	ng	4847680	3	9.898	5558330	20.0
t-Butylhydroqui...	10.110	27.9	ng	7744420	3	9.898	5558330	20.0
Dodecanoic acid	10.463	1649.9	ng	458539000	3	9.898	5558330	20.0
Tetradecanoic acid	11.221	20.0	ng	139713000	4	11.392	139713000	20.0
n-Hexadecanoic ...	12.010	12.3	ng	85541300	4	11.392	139713000	20.0
6-Octadecenoic ...	12.721	208.6	ng	106260000	5	14.033	10186800	20.0
Octadecanoic acid	12.774	44.7	ng	22751700	5	14.033	10186800	20.0
Benzoic acid, t...	12.933	9.5	ng	4836290	5	14.033	10186800	20.0
Oxiraneoctanoic...	15.198	20.0	ng	4732130	6	15.515	4732130	20.0