

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
 Data File : BF128239.D
 Acq On : 13 May 2022 15:15
 Operator : CG\JU
 Sample : N2823-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SC-2

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-BF050922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128239.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.510	544	548	563	rBV	901913	1627944	13.53%	4.220%
2	5.875	599	610	612	rBV	2452912	4595372	38.20%	11.913%
3	6.522	715	720	729	rBV	1285947	1656777	13.77%	4.295%
4	6.728	745	755	765	rVB	90404	165834	1.38%	0.430%
5	6.887	778	782	785	rBV	432632	389990	3.24%	1.011%
6	6.963	787	795	798	rBV	4455745	6887075	57.24%	17.853%
7	7.293	844	851	863	rVB	316019	261304	2.17%	0.677%
8	7.422	870	873	875	rBV	269686	253281	2.11%	0.657%
9	7.451	875	878	881	rVB	1209685	1068920	8.88%	2.771%
10	8.169	996	1000	1003	rBV	613333	505398	4.20%	1.310%
11	9.245	1177	1183	1186	rBV	2184763	1934669	16.08%	5.015%
12	9.922	1295	1298	1302	rVB	623041	565968	4.70%	1.467%
13	10.716	1429	1433	1437	rBV	1322801	1167500	9.70%	3.027%
14	10.828	1447	1452	1455	rBV	184867	226008	1.88%	0.586%
15	11.263	1523	1526	1529	rBV	282652	226517	1.88%	0.587%
16	11.416	1548	1552	1555	rBV	697543	605037	5.03%	1.568%
17	13.004	1818	1822	1825	rVB	1728603	1503599	12.50%	3.898%
18	13.480	1899	1903	1907	rVB	413149	454816	3.78%	1.179%
19	13.563	1914	1917	1920	rVB	134236	130682	1.09%	0.339%
20	14.051	1993	2000	2003	rBV	7429163	12031010	100.00%	31.188%
21	15.557	2252	2256	2263	rVB	314411	427000	3.55%	1.107%
22	16.263	2372	2376	2390	rVB	202805	448084	3.72%	1.162%
23	16.568	2423	2428	2434	rVB	434210	721872	6.00%	1.871%
24	16.710	2447	2452	2460	rVB2	245578	457870	3.81%	1.187%
25	17.104	2515	2519	2531	rVB	126913	263084	2.19%	0.682%

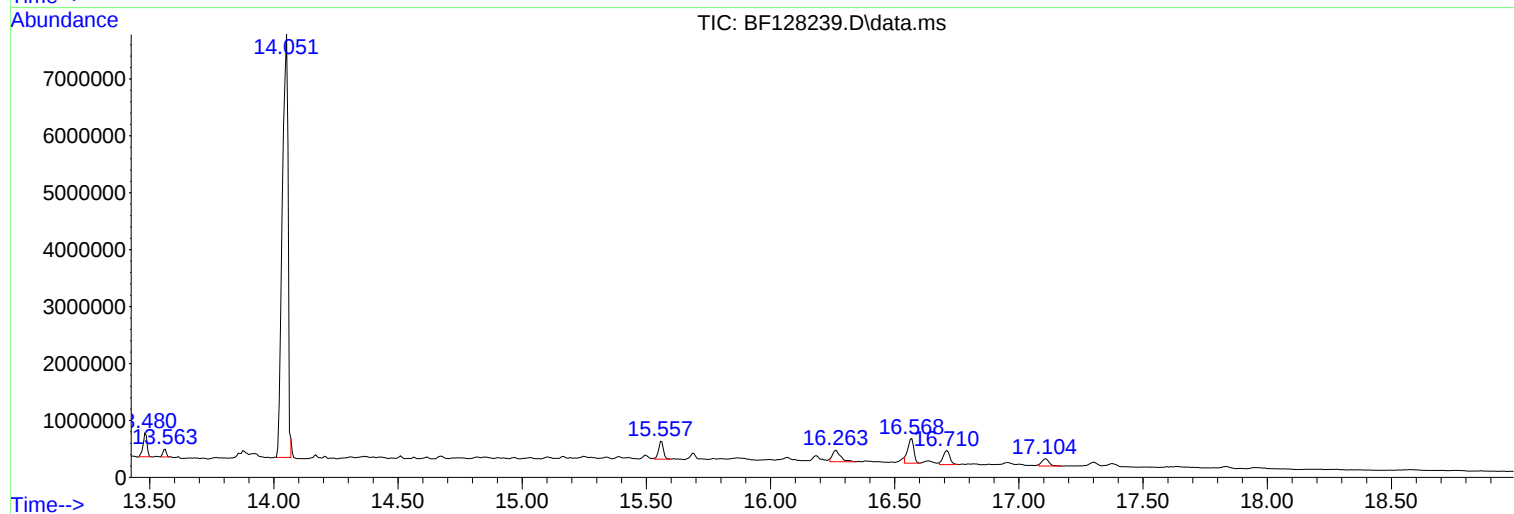
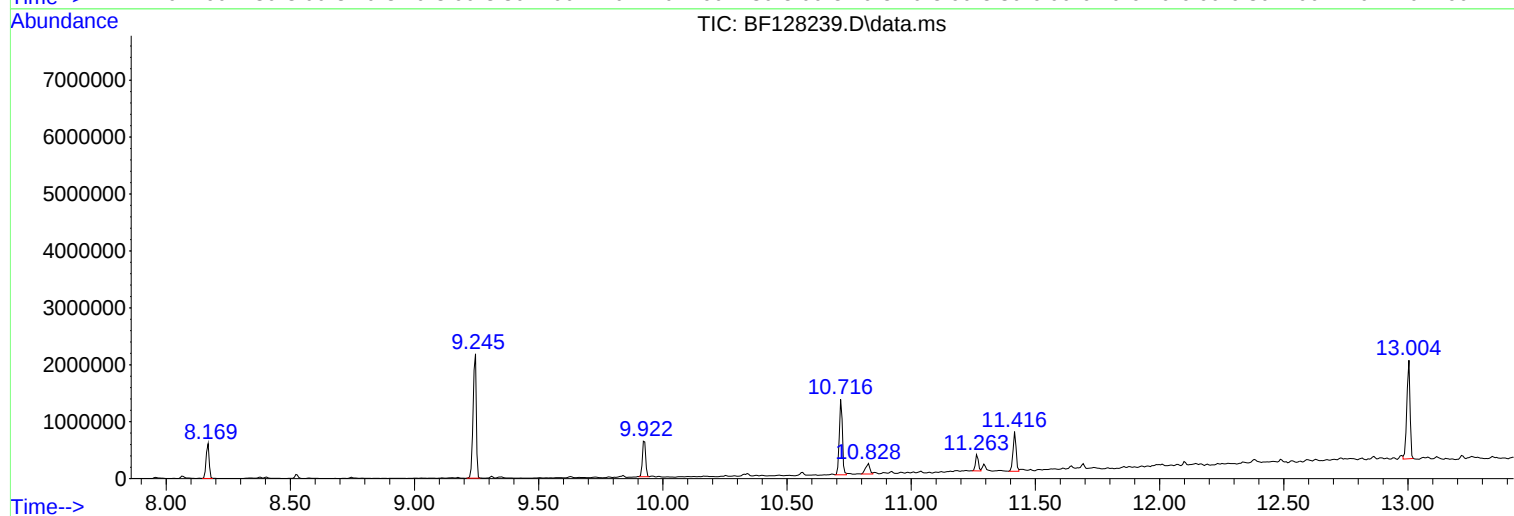
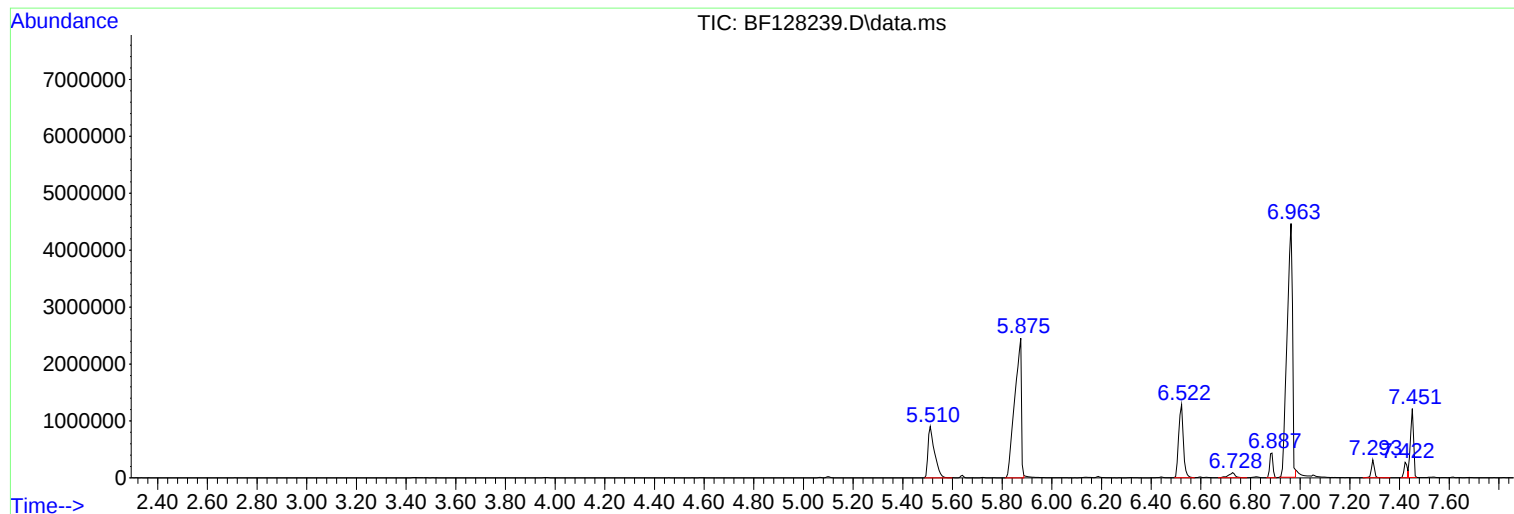
Sum of corrected areas: 38575611

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-2

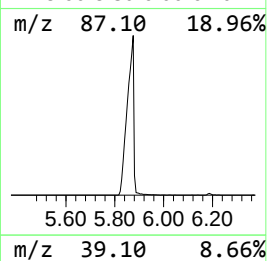
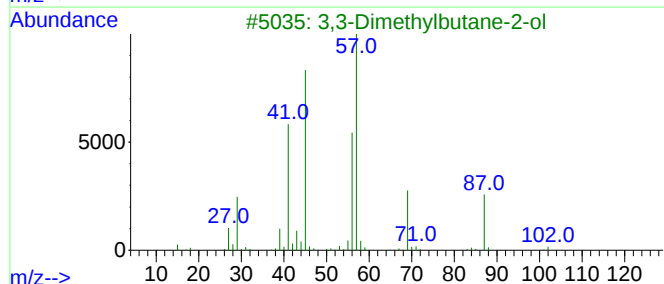
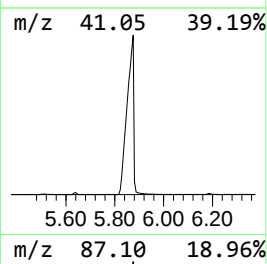
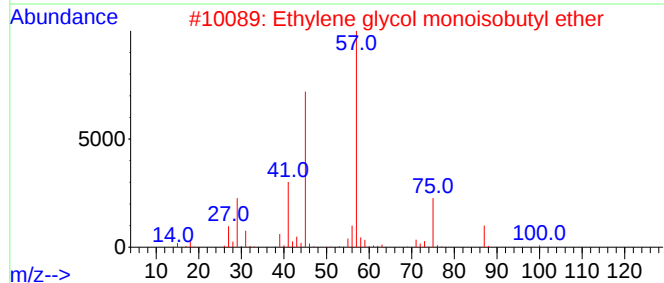
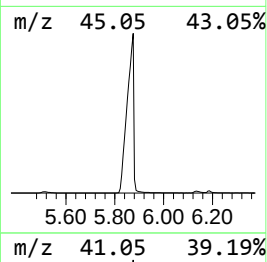
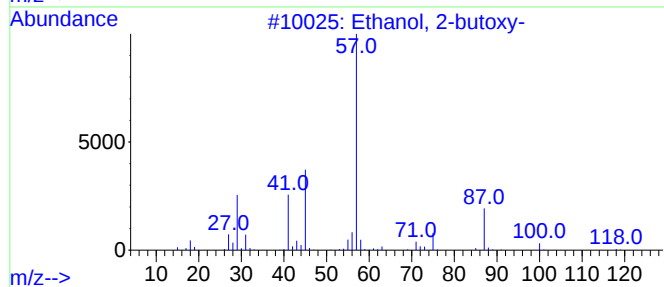
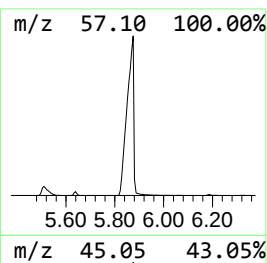
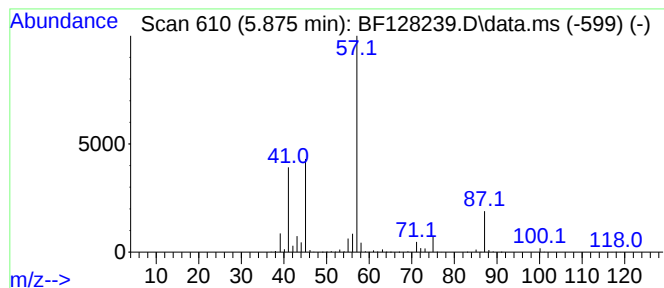
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.875	235.67 ng	4595370	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	40
4			Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	17
5			1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-2

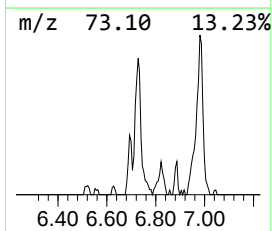
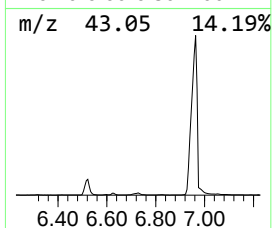
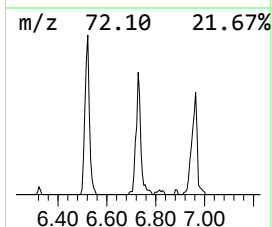
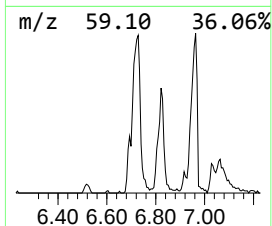
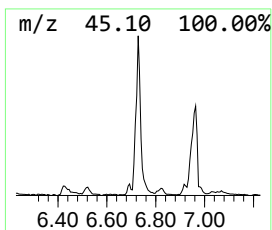
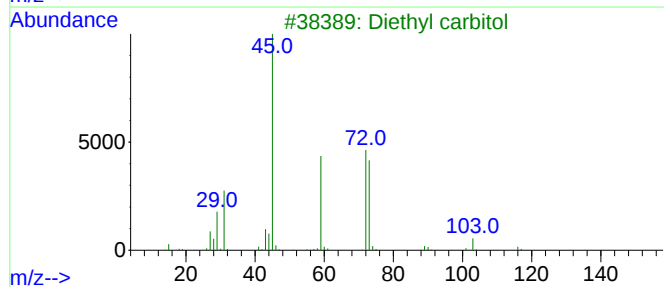
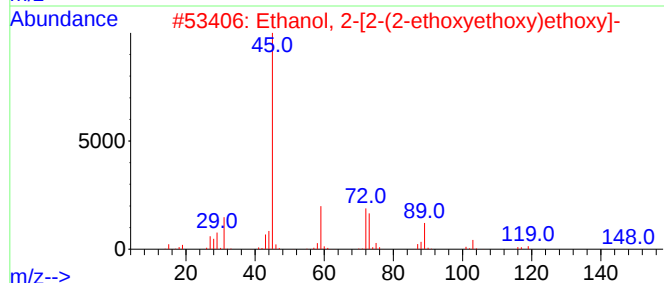
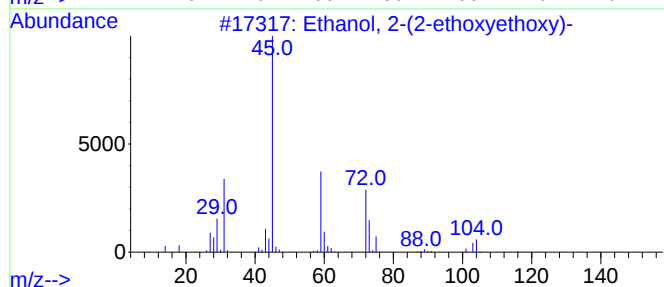
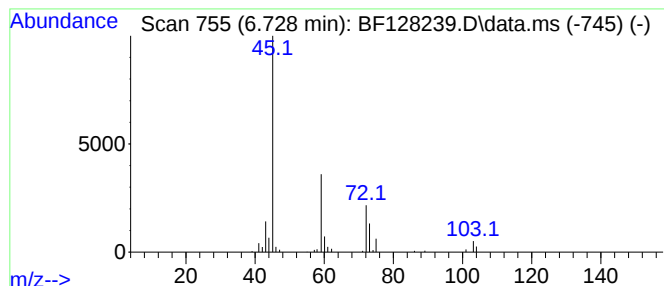
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.728	8.50 ng	165834	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	72
3			Diethyl carbitol	162	C8H18O3	000112-36-7	47
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-2

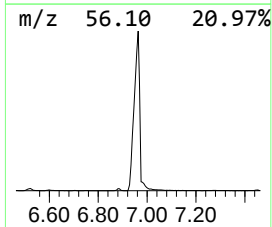
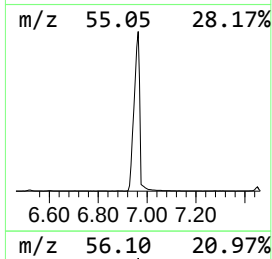
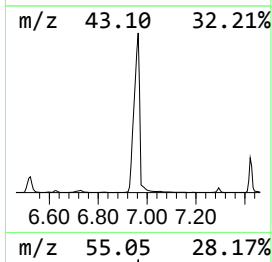
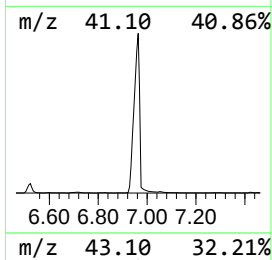
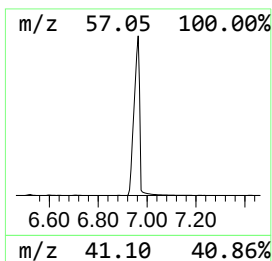
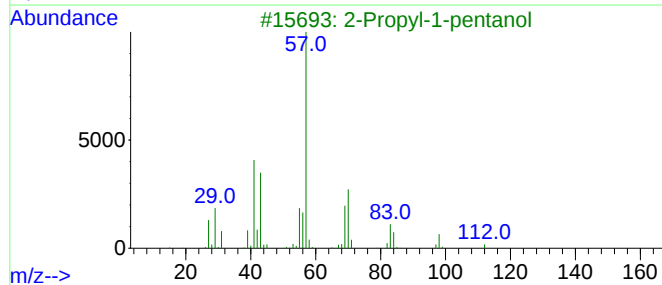
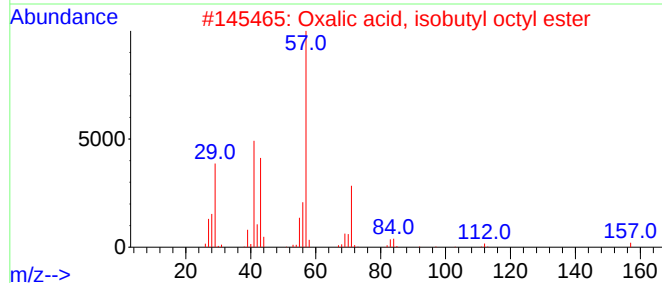
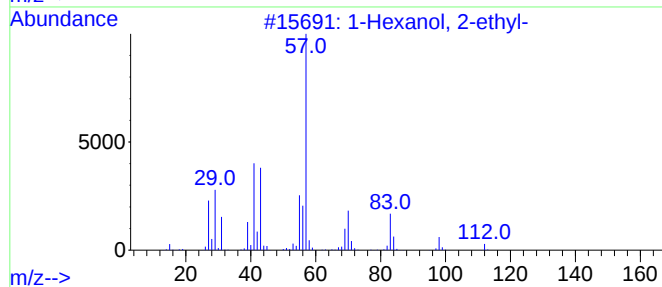
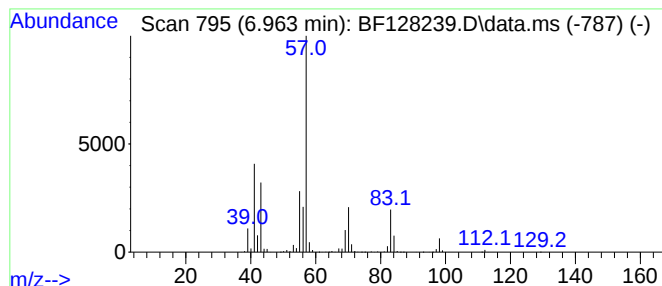
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.963	353.19 ng	6887080	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	45
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-2

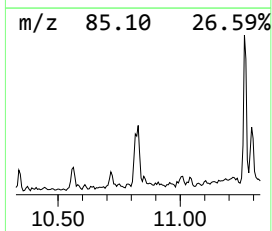
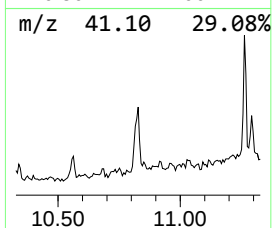
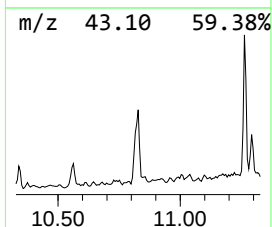
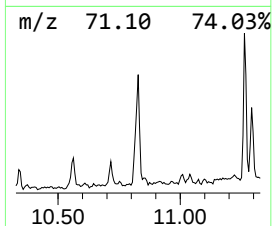
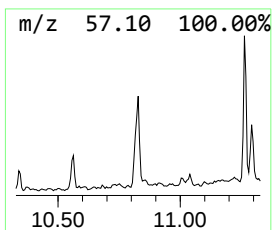
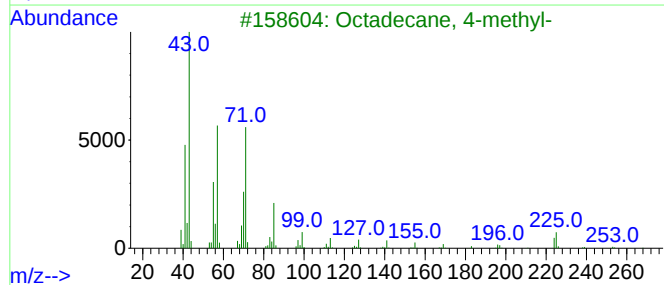
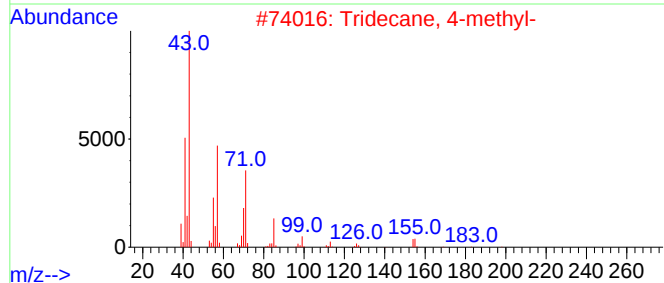
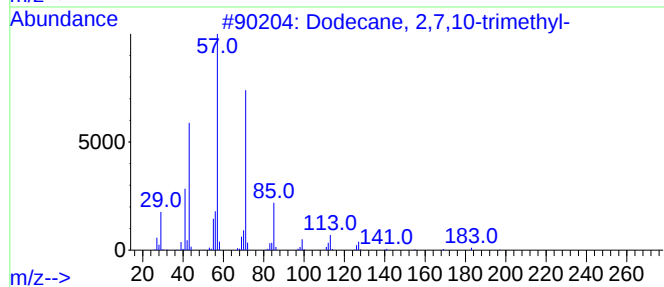
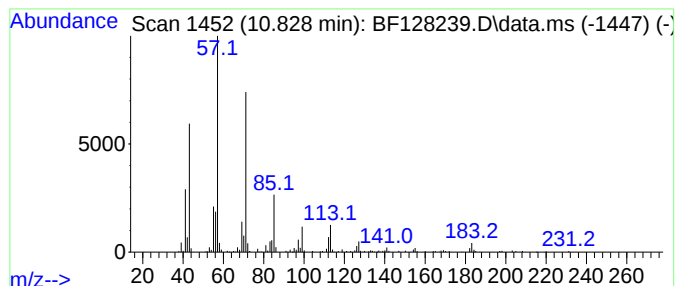
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Dodecane, 2,7,10-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.828	7.47 ng	226008	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
2			Tridecane, 4-methyl-	198	C14H30	026730-12-1	83
3			Octadecane, 4-methyl-	268	C19H40	010544-95-3	78
4			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	72
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-2

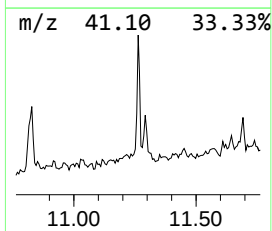
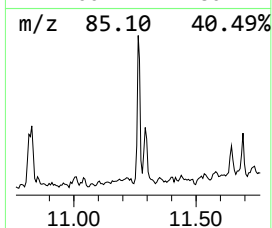
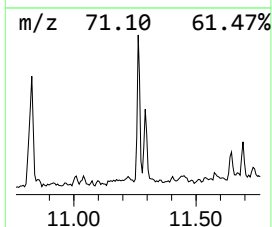
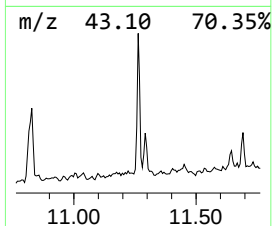
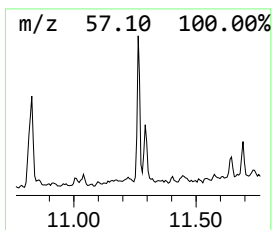
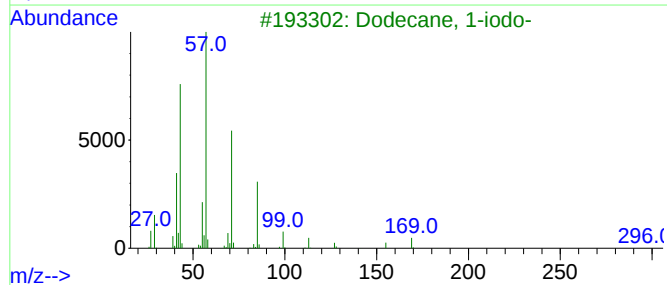
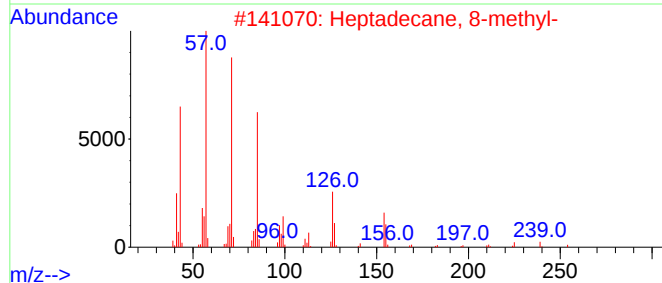
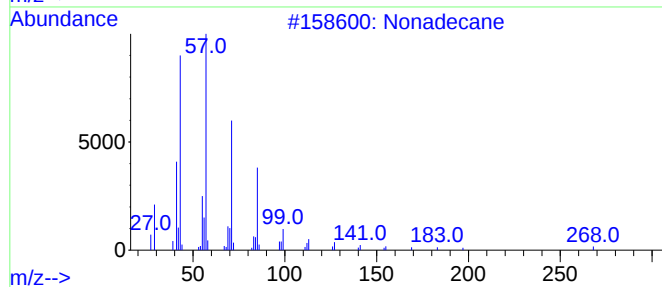
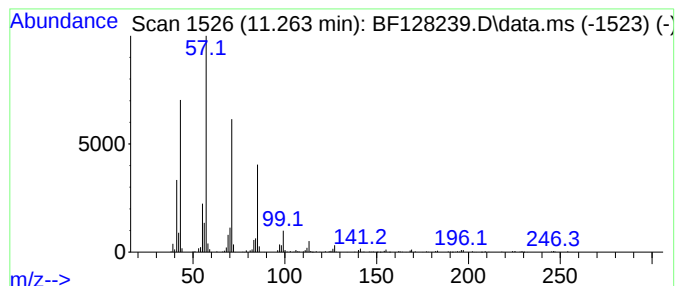
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.263	7.49 ng	226517	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Heptadecane, 8-methyl-	254	C18H38	013287-23-5	87
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
4			Hexadecane	226	C16H34	000544-76-3	80
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-2

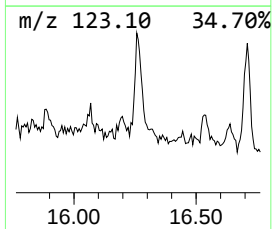
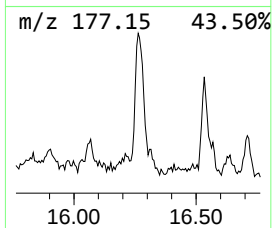
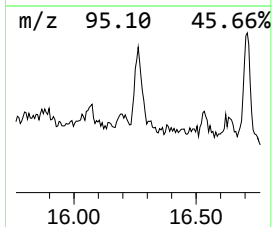
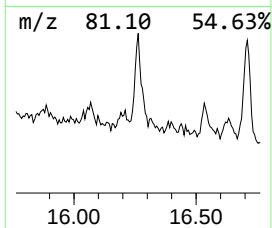
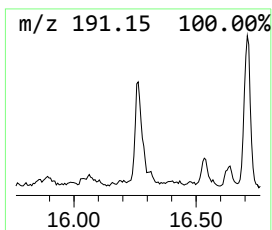
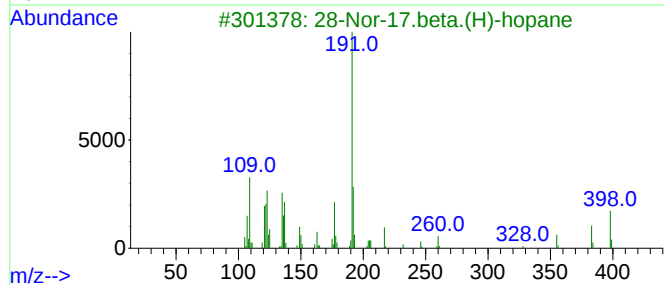
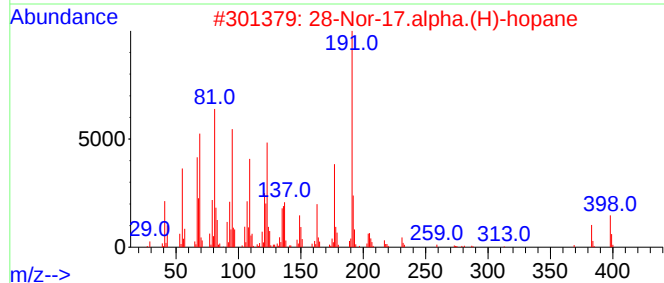
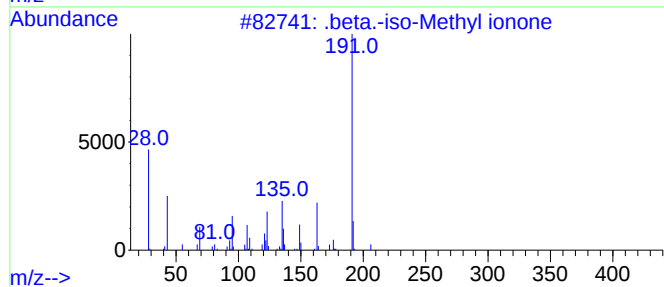
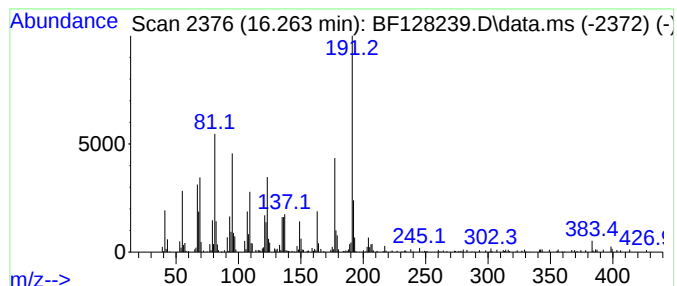
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 .beta.-iso-Methyl ionone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	20.99 ng	448084	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	58
2			28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	50
3			28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	45
4			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
5			2,3,4,5-Tetramethylacetanilide	191	C12H17NO	1000432-93-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-2

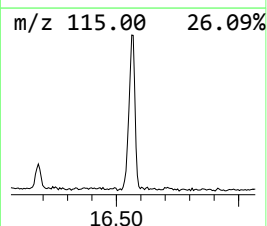
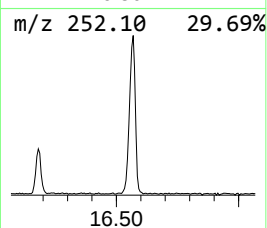
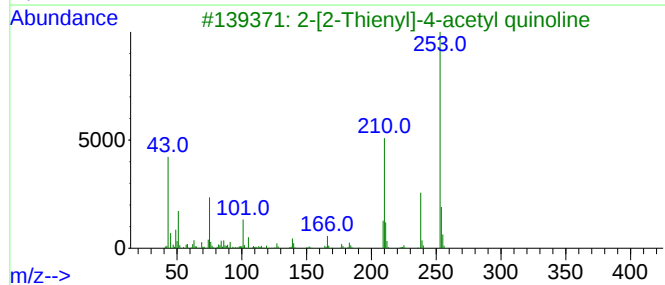
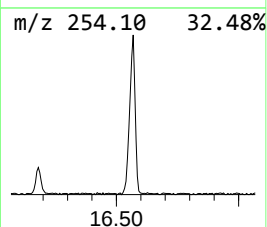
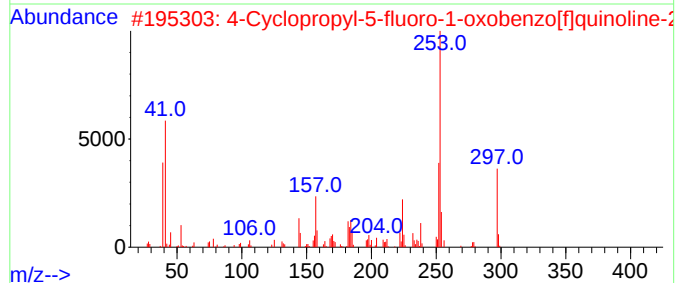
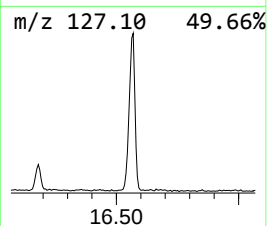
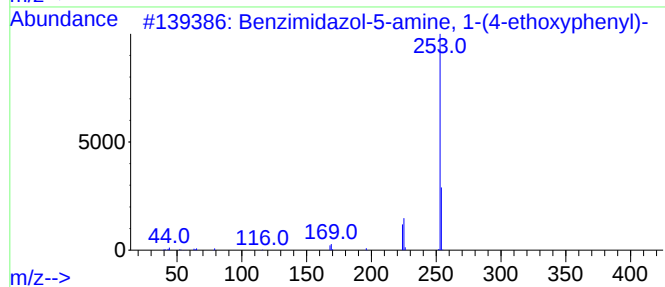
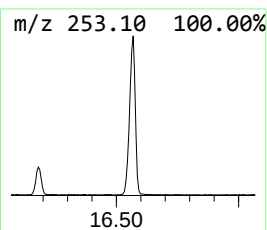
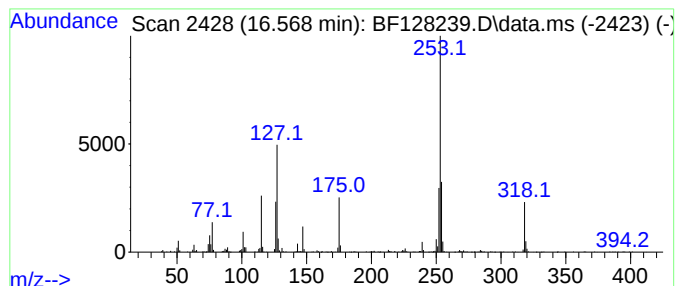
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.568 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.568	33.81 ng	721872	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzimidazol-5-amine, 1-(4-ethox...	253	C15H15N3O	007104-62-3	27
2			4-Cyclopropyl-5-fluoro-1-oxobenz...	297	C17H12FNO3	1000435-59-2	17
3			2-[2-Thienyl]-4-acetyl quinoline	253	C15H11NOS	027302-83-6	12
4			9,10[1',2']-Benzenoanthracene, 9...	254	C20H14	000477-75-8	11
5			2-Anilino-4-chloroquinoline	254	C15H11ClN2	032888-95-2	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

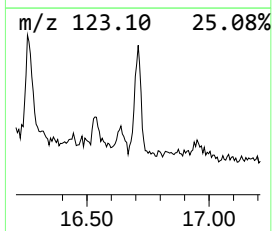
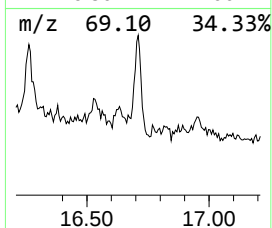
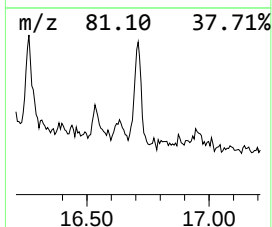
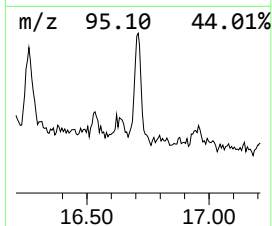
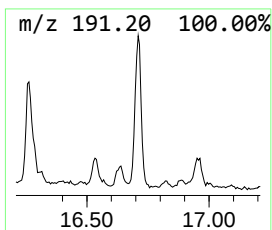
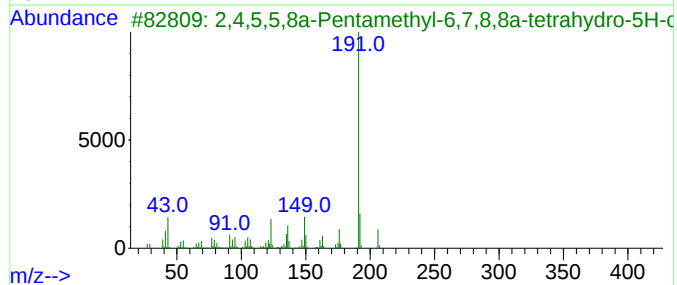
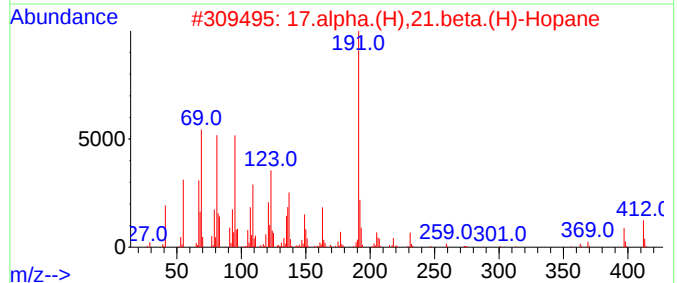
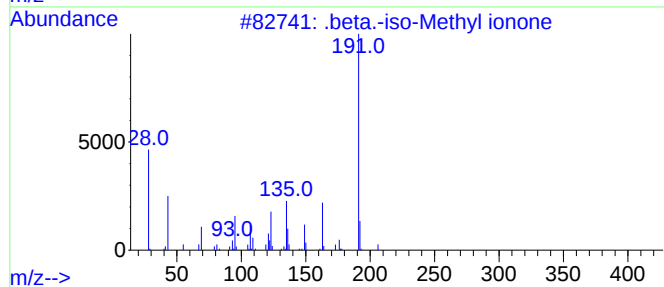
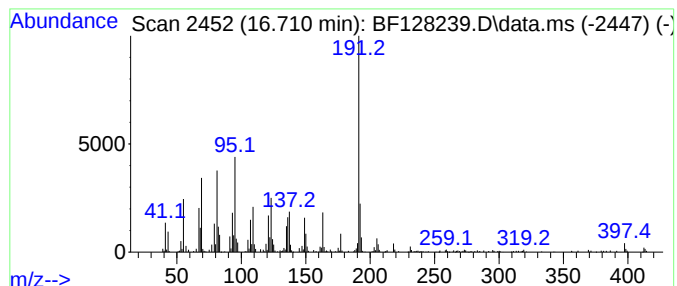
Instrument :
BNA_F
ClientSampleId :
SC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.710	21.45 ng	457870	Perylene-d12	15.563	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	72
2	17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	64
3	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	40
4	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	40
5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-2

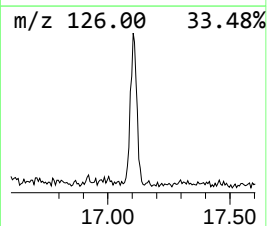
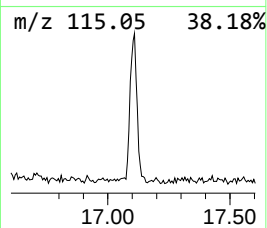
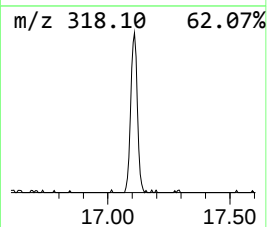
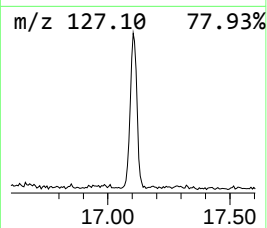
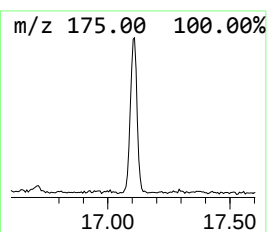
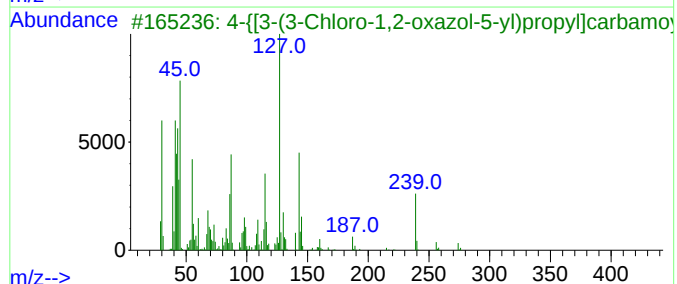
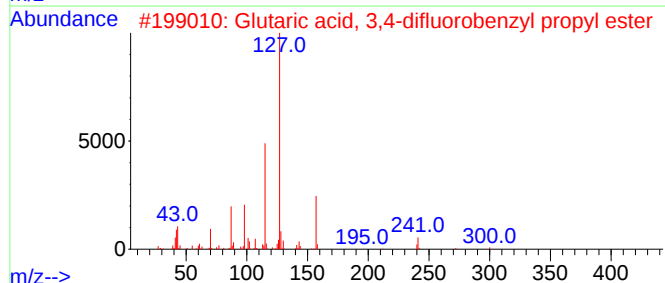
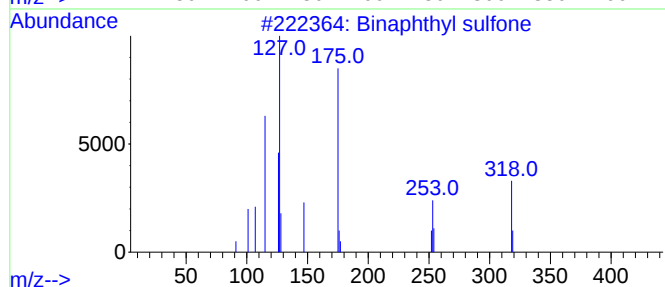
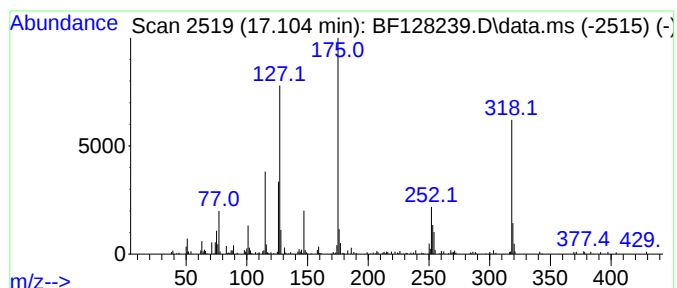
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Binaphthyl sulfone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.104	12.32 ng	263084	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Binaphthyl sulfone	318	C20H14O2S	032390-26-4	52
2			Glutaric acid, 3,4-difluorobenzy...	300	C15H18F2O4	1000377-63-3	25
3			4-([3-(3-Chloro-1,2-oxazol-5-yl)...	274	C11H15ClN2O4	1000443-54-1	22
4			4-Methyl-2,5-quinolindiol	175	C10H9NO2	131195-67-0	14
5			4-Methyl-2,6-dihydroxyquinoline	175	C10H9NO2	034982-01-9	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051322\
Data File : BF128239.D
Acq On : 13 May 2022 15:15
Operator : CG\JU
Sample : N2823-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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
Ethanol, 2-butoxy-	5.875	235.7	ng	4595370	1	6.887	389990	20.0
Ethanol, 2-(2-e...	6.728	8.5	ng	165834	1	6.887	389990	20.0
1-Hexanol, 2-et...	6.963	353.2	ng	6887080	1	6.887	389990	20.0
Dodecane, 2,7,1...	10.828	7.5	ng	226008	4	11.416	605037	20.0
Nonadecane	11.263	7.5	ng	226517	4	11.416	605037	20.0
.beta.-iso-Meth...	16.262	21.0	ng	448084	6	15.563	427000	20.0
unknown16.568	16.568	33.8	ng	721872	6	15.563	427000	20.0
17.alpha.(H),21...	16.710	21.4	ng	457870	6	15.563	427000	20.0
Binaphthyl sulfone	17.104	12.3	ng	263084	6	15.563	427000	20.0