

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
 Data File : BF125823.D
 Acq On : 13 Oct 2021 13:11
 Operator : JU/CG
 Sample : M4127-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHRT-27051

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-BF100721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125823.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	1223426	1208180	35.72%	4.420%
2	5.063	496	506	513	rBV	38517	50734	1.50%	0.186%
3	5.463	569	574	577	rBV	3459026	3319196	98.14%	12.142%
4	6.469	740	745	748	rBV	3412112	3213940	95.03%	11.757%
5	6.845	805	809	812	rBV	1184112	998000	29.51%	3.651%
6	7.398	899	903	907	rBV	2153048	2093776	61.91%	7.659%
7	8.022	1006	1009	1018	rBV	594911	528004	15.61%	1.931%
8	8.122	1022	1026	1029	rBV	1702338	1329310	39.31%	4.863%
9	9.198	1205	1209	1212	rBV	4238303	3381985	100.00%	12.371%
10	9.875	1320	1324	1328	rBV	1776918	1420612	42.01%	5.197%
11	10.663	1454	1458	1461	rBV	2285937	1983832	58.66%	7.257%
12	11.363	1573	1577	1579	rBV	1224487	1073449	31.74%	3.927%
13	11.886	1663	1666	1669	rBV2	632393	578463	17.10%	2.116%
14	12.192	1716	1718	1721	rBV3	168869	144142	4.26%	0.527%
15	12.410	1752	1755	1759	rVB	315169	298303	8.82%	1.091%
16	12.674	1797	1800	1804	rBV2	651091	624369	18.46%	2.284%
17	12.798	1819	1821	1824	rVB	187352	149487	4.42%	0.547%
18	12.945	1842	1846	1849	rVB	2497355	2109774	62.38%	7.718%
19	13.127	1875	1877	1882	rVB3	147402	154841	4.58%	0.566%
20	13.992	2020	2024	2027	rBV	1169782	1141787	33.76%	4.177%
21	15.027	2196	2200	2202	rBV	96239	139725	4.13%	0.511%
22	15.321	2248	2250	2255	rVB	72719	89323	2.64%	0.327%
23	15.386	2258	2261	2265	rVB	79338	80601	2.38%	0.295%
24	15.451	2267	2272	2276	rBV	996702	1175762	34.77%	4.301%
25	15.921	2349	2352	2358	rVB2	36298	49390	1.46%	0.181%

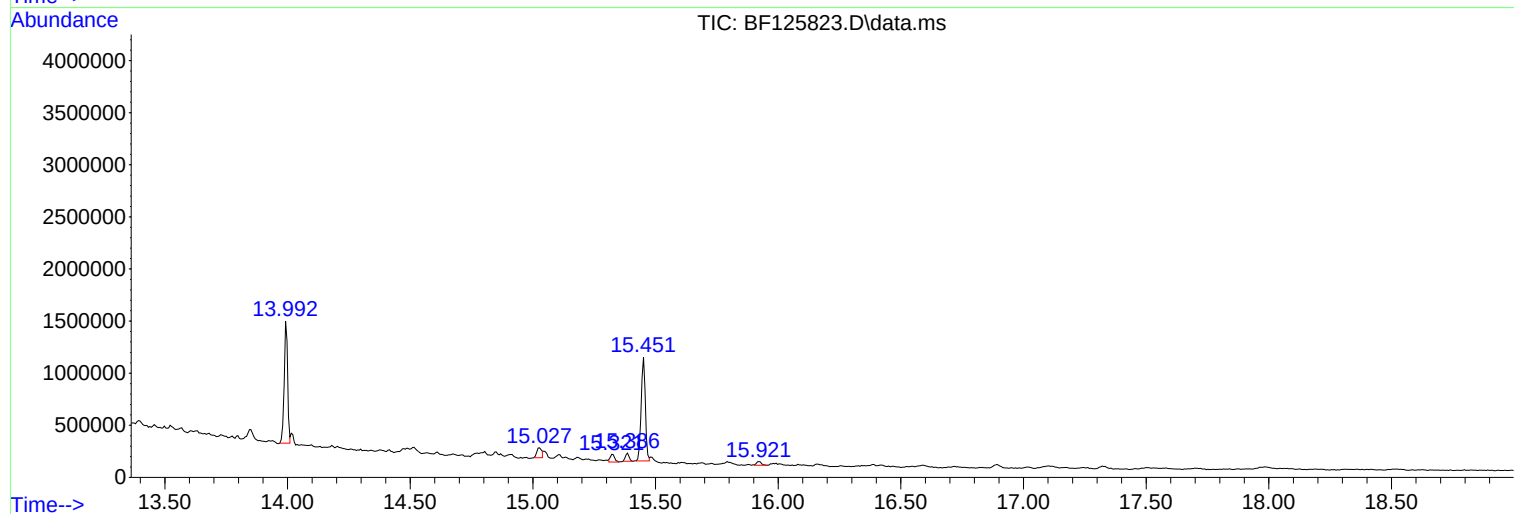
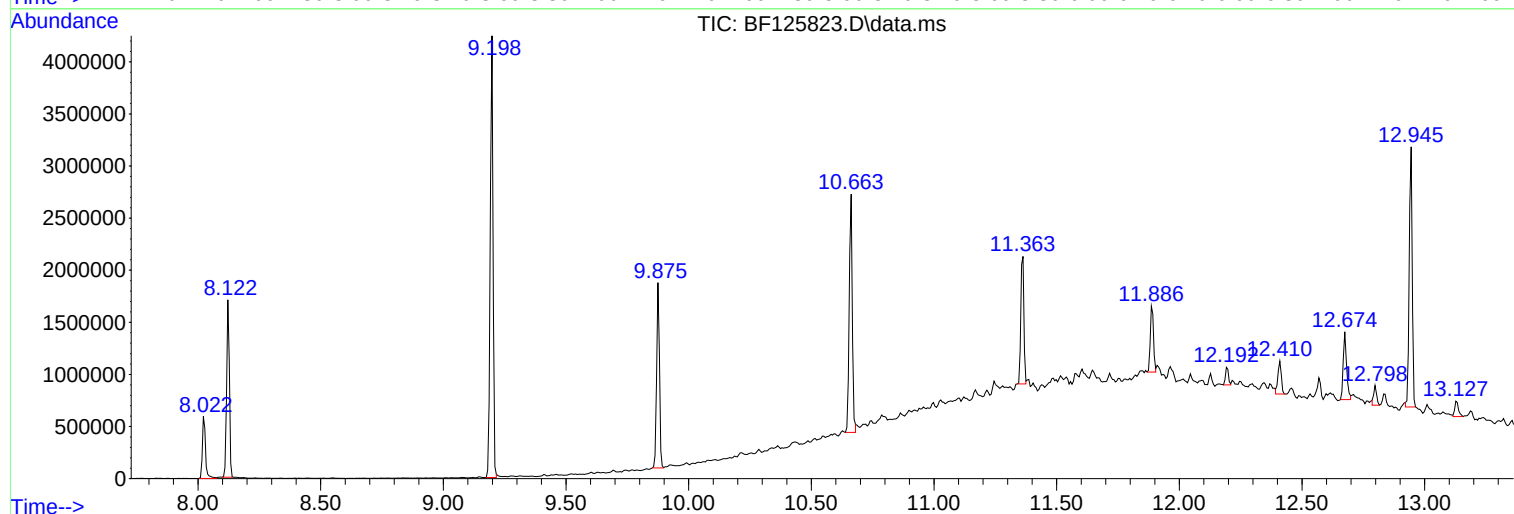
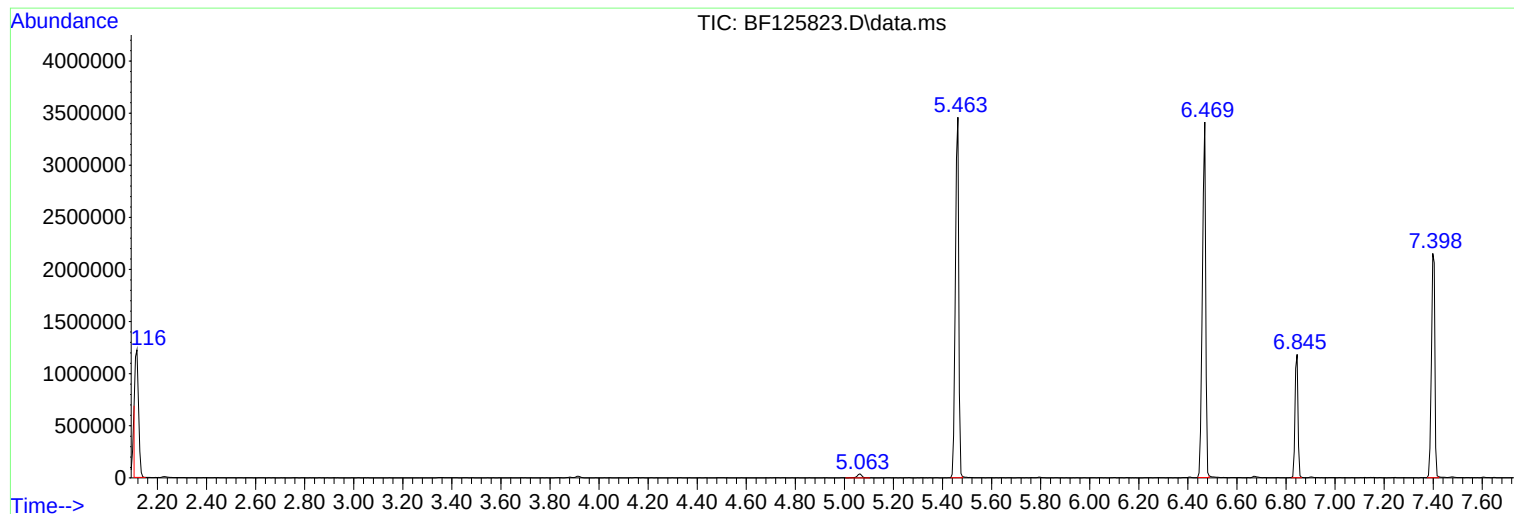
Sum of corrected areas: 27336985

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125823.D
Acq On : 13 Oct 2021 13:11
Operator : JU/CG
Sample : M4127-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-27051

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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\BF101321\
Data File : BF125823.D
Acq On : 13 Oct 2021 13:11
Operator : JU/CG
Sample : M4127-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-27051

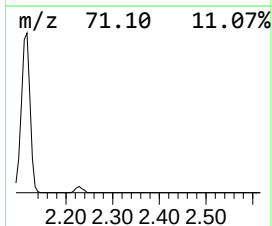
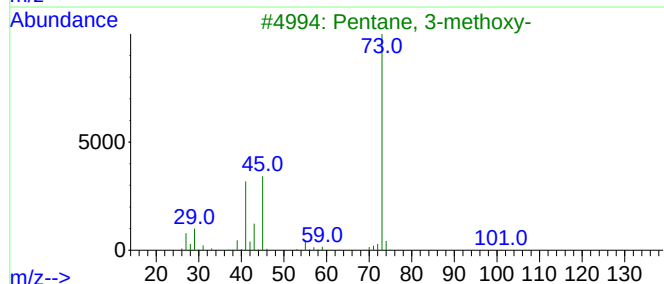
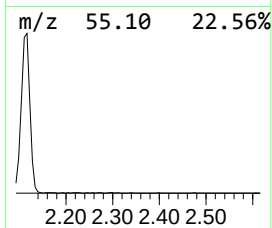
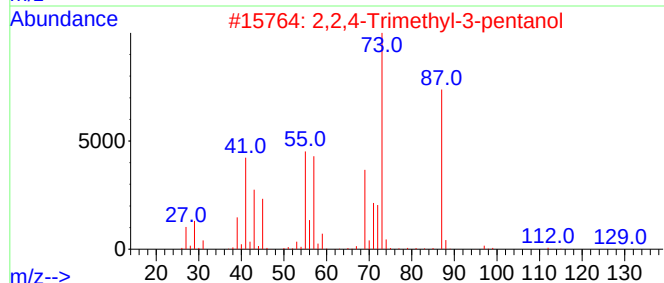
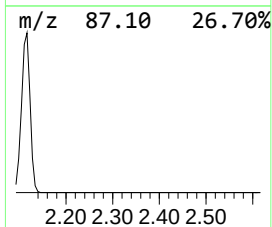
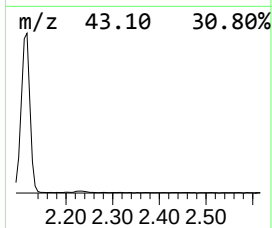
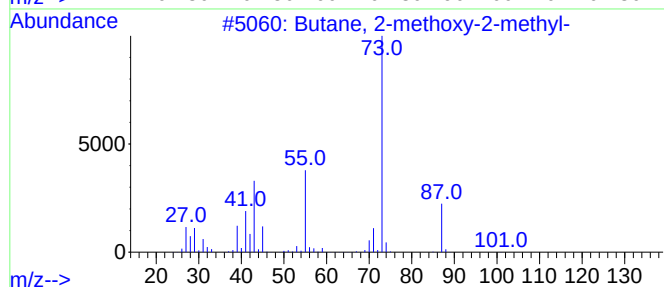
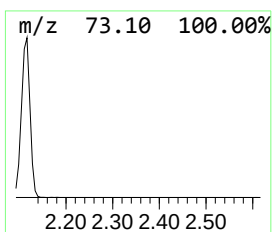
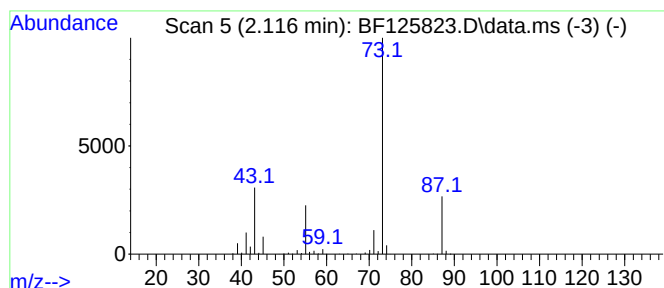
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	24.21 ng	1208180	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125823.D
Acq On : 13 Oct 2021 13:11
Operator : JU/CG
Sample : M4127-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-27051

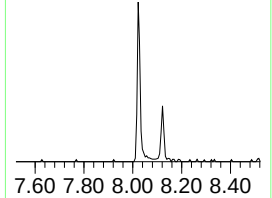
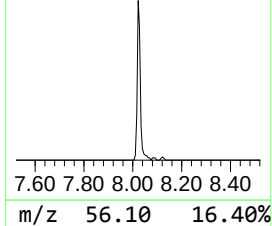
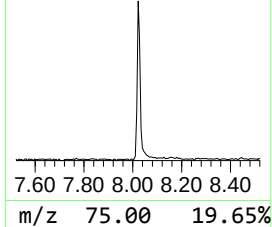
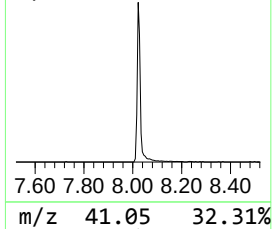
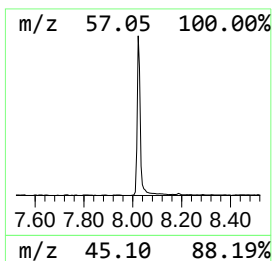
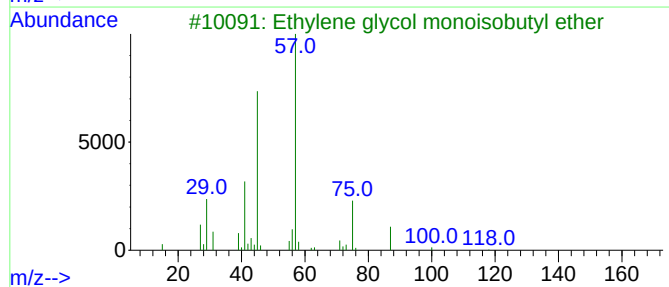
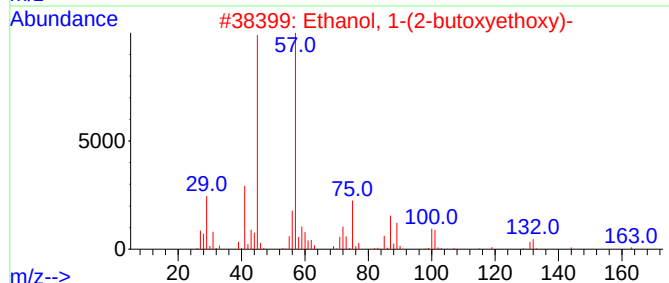
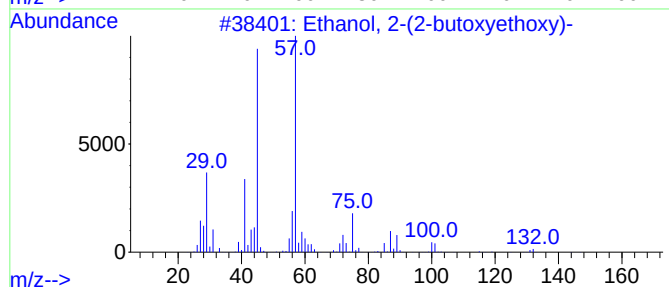
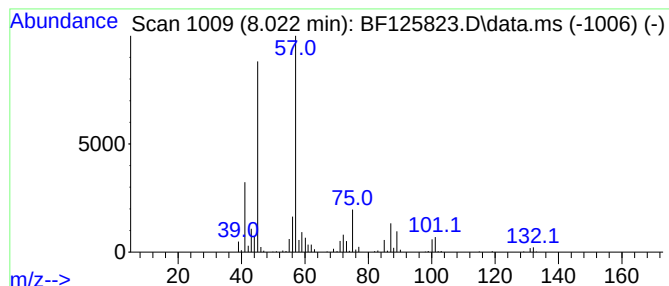
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	7.94 ng	528004	Naphthalene-d8	8.122

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			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125823.D
Acq On : 13 Oct 2021 13:11
Operator : JU/CG
Sample : M4127-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-27051

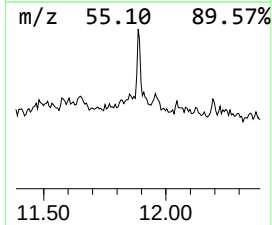
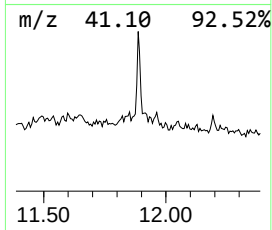
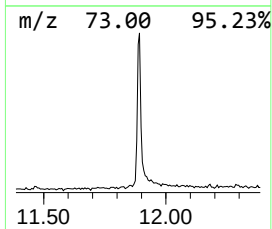
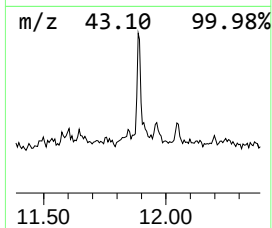
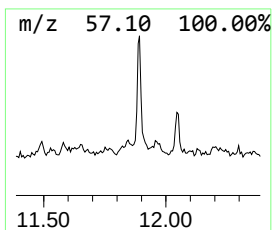
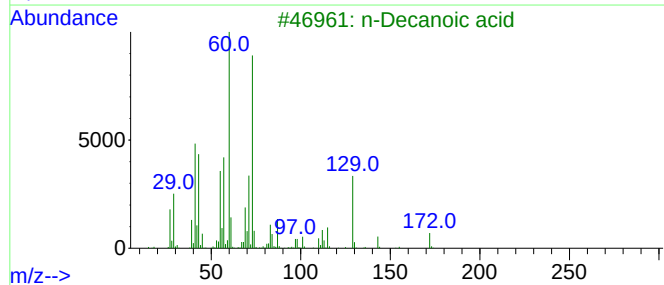
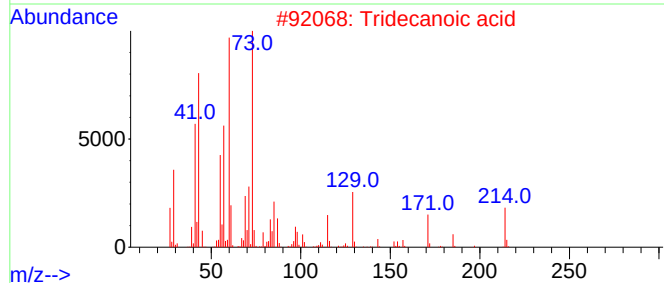
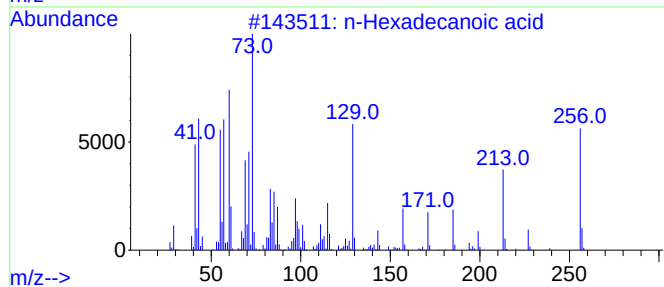
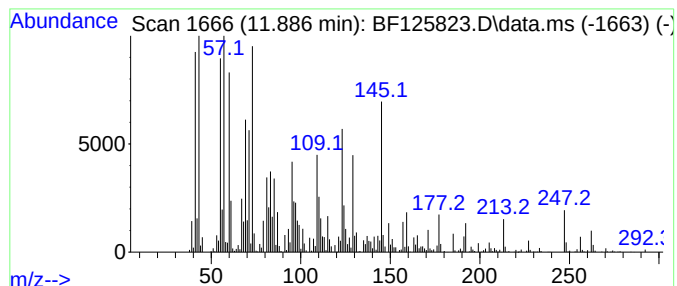
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	10.78 ng	578463	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	38
3			n-Decanoic acid	172	C10H20O2	000334-48-5	30
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	30
5			Octadecanoic acid	284	C18H36O2	000057-11-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125823.D
Acq On : 13 Oct 2021 13:11
Operator : JU/CG
Sample : M4127-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

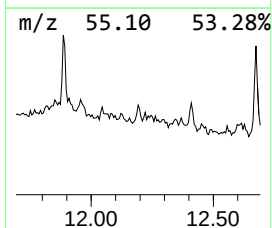
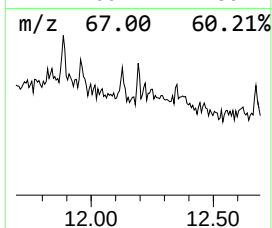
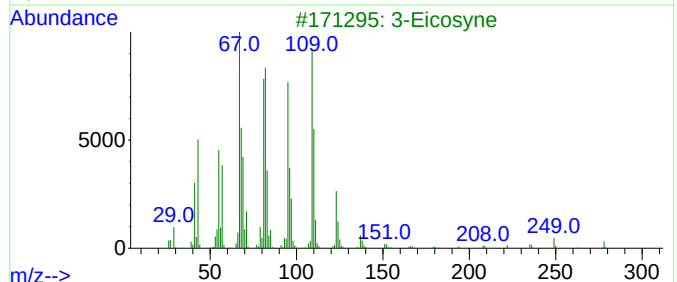
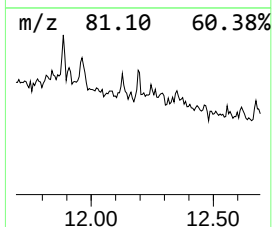
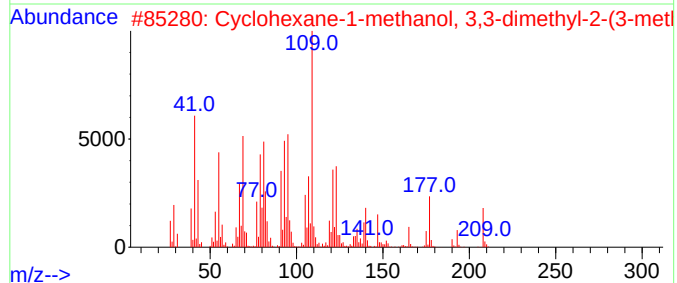
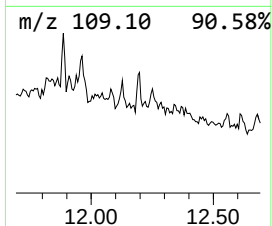
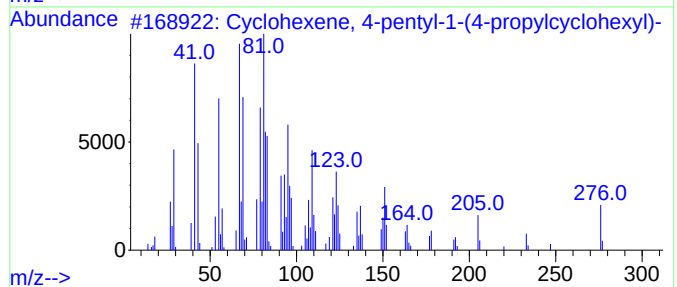
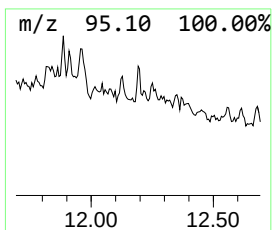
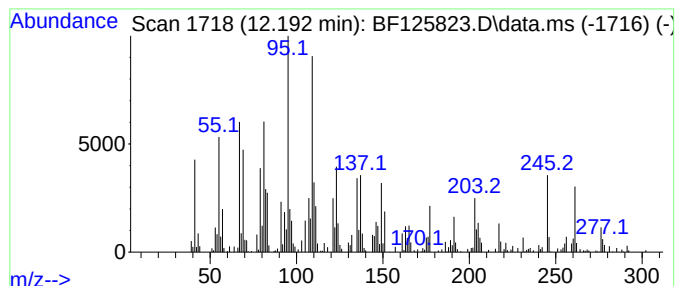
Instrument :
BNA_F
ClientSampleId :
CHRT-27051

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclohexene, 4-pentyl-1-(4-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.192	2.69 ng	144142	Phenanthrene-d10		11.363	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexene, 4-pentyl-1-(4-propy...		276	C20H36	108067-17-0	56
2	Cyclohexane-1-methanol, 3,3-dime...		208	C14H24O	1000196-01-5	46
3	3-Eicosyne		278	C20H38	061886-66-6	44
4	1H-Naphtho[2,1-b]pyran, 4a,5,6,6...		262	C18H30O	005153-92-4	43
5	4-Methylimidazole-5-butyric acid		168	C8H12N2O2	1000129-14-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125823.D
Acq On : 13 Oct 2021 13:11
Operator : JU/CG
Sample : M4127-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-27051

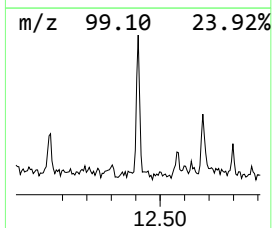
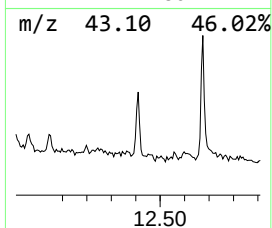
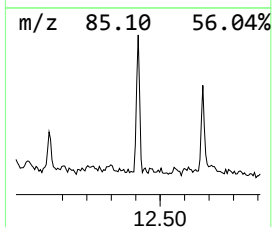
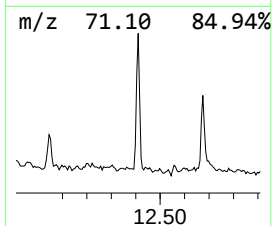
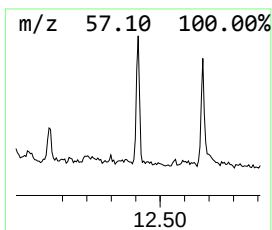
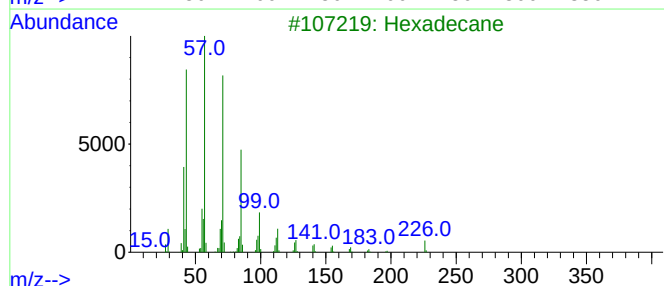
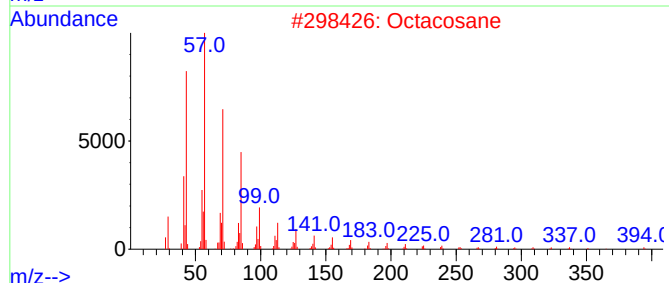
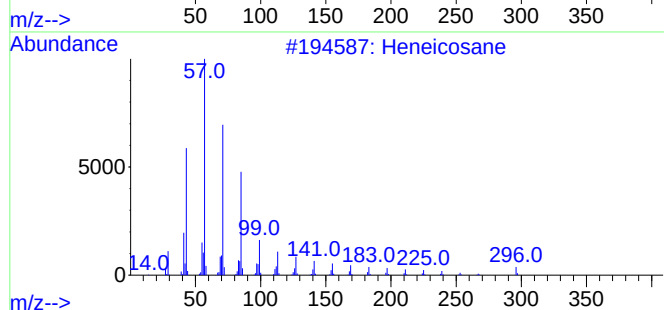
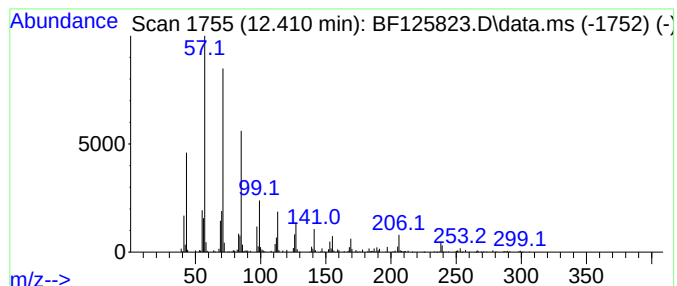
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	5.56 ng	298303	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Octacosane	394	C28H58	000630-02-4	86
3			Hexadecane	226	C16H34	000544-76-3	86
4			Eicosane, 2-methyl-	296	C21H44	001560-84-5	86
5			Triacontane	422	C30H62	000638-68-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125823.D
Acq On : 13 Oct 2021 13:11
Operator : JU/CG
Sample : M4127-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-27051

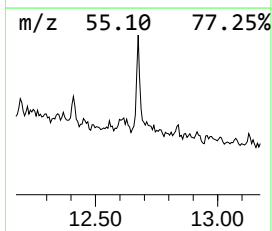
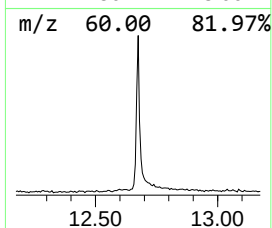
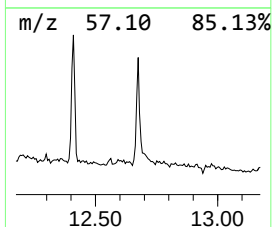
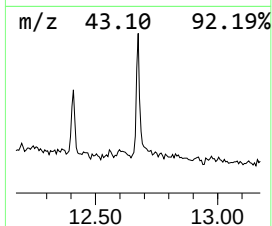
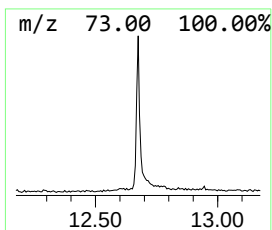
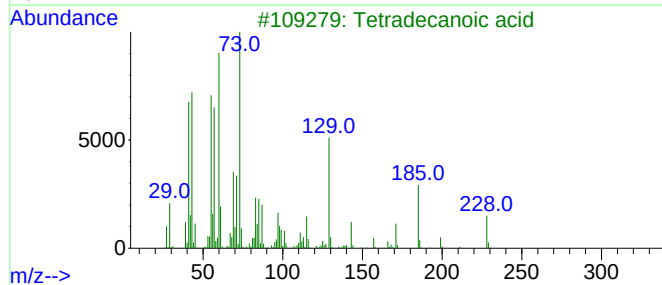
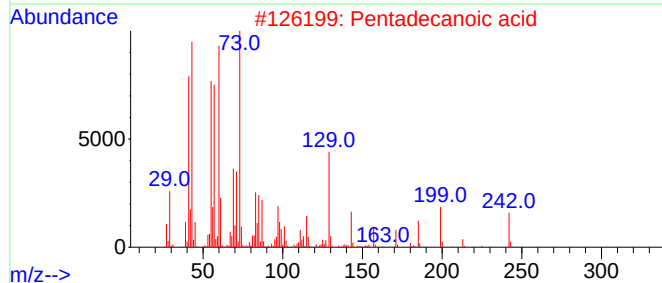
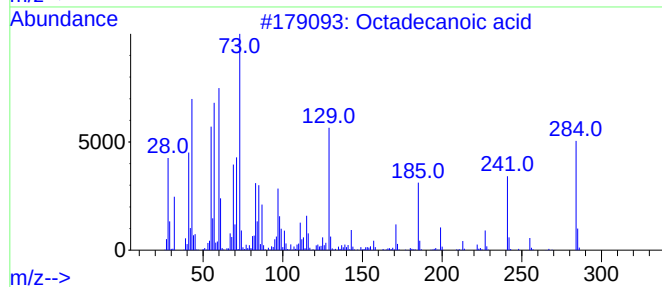
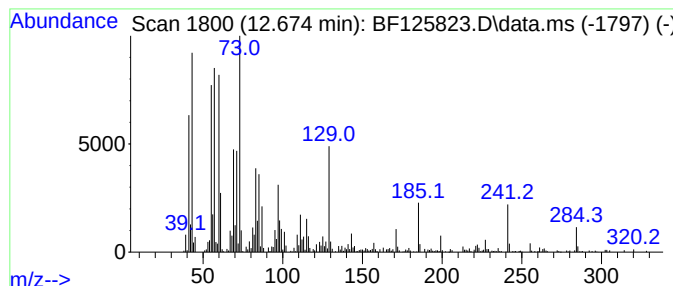
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	11.63 ng	624369	Phenanthrene-d10	11.363

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125823.D
Acq On : 13 Oct 2021 13:11
Operator : JU/CG
Sample : M4127-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-27051

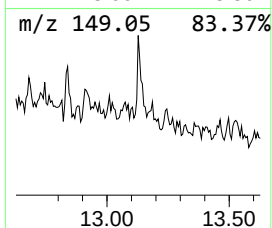
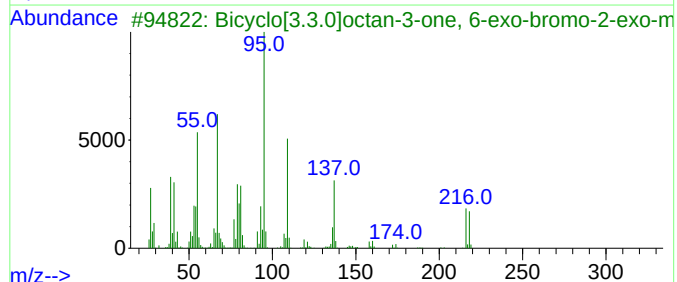
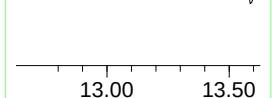
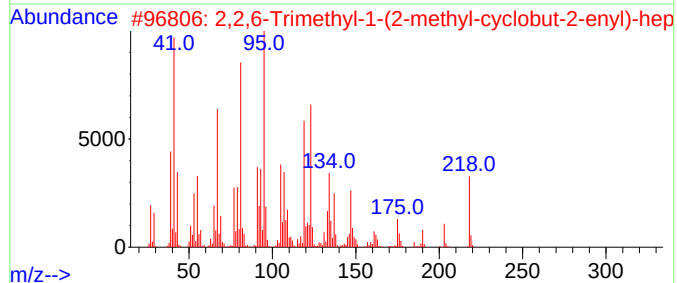
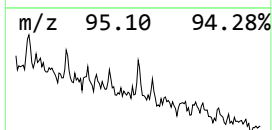
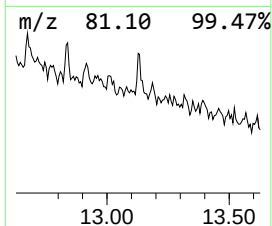
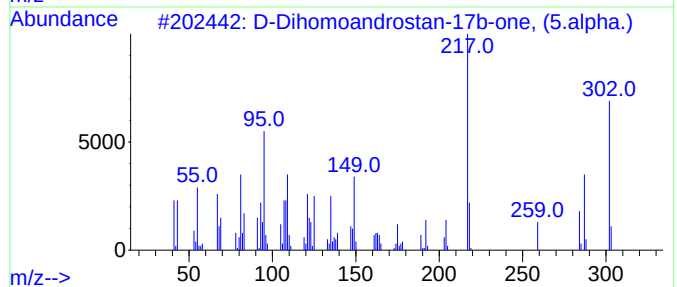
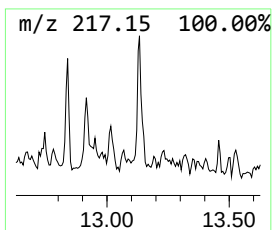
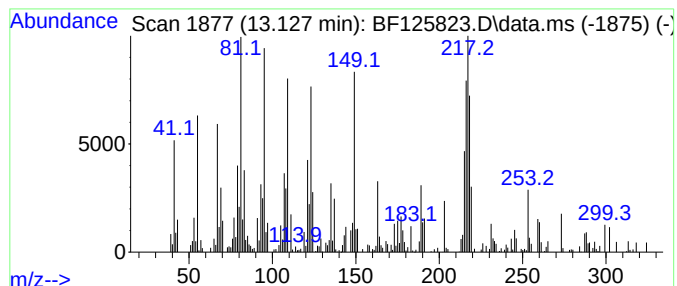
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.127 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.127	2.71 ng	154841	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Dihomoandrostan-17b-one, (5.alpha...	302	C21H34O	032319-07-6	42
2			2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	38
3			Bicyclo[3.3.0]octan-3-one, 6-exo...	216	C9H13BrO	1000149-28-6	35
4			6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	35
5			Androstane	260	C19H32	024887-75-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125823.D
Acq On : 13 Oct 2021 13:11
Operator : JU/CG
Sample : M4127-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-27051

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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
Butane, 2-metho...	2.116	24.2	ng	1208180	1	6.845	998000	20.0
Ethanol, 2-(2-b...	8.022	7.9	ng	528004	2	8.122	1329310	20.0
n-Hexadecanoic ...	11.886	10.8	ng	578463	4	11.363	1073450	20.0
Cyclohexene, 4-...	12.192	2.7	ng	144142	4	11.363	1073450	20.0
Heneicosane	12.410	5.6	ng	298303	4	11.363	1073450	20.0
Octadecanoic acid	12.674	11.6	ng	624369	4	11.363	1073450	20.0
unknown13.127	13.127	2.7	ng	154841	5	13.992	1141790	20.0