

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
 Data File : BF125545.D
 Acq On : 21 Sep 2021 20:12
 Operator : JU/CG
 Sample : M3835-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-CB-03-(1.0)

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-BF092121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125545.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	28	rVB	2825013	3814554	72.26%	11.588%
2	5.210	527	531	535	rVB	448801	402349	7.62%	1.222%
3	5.504	577	581	585	rBV	2078226	1923407	36.43%	5.843%
4	6.504	747	751	756	rBV	1433037	1176637	22.29%	3.575%
5	6.898	814	818	823	rVB	1050088	973768	18.45%	2.958%
6	7.451	907	912	915	rBV	2592507	2694203	51.03%	8.185%
7	7.569	929	932	935	rBV	89602	67940	1.29%	0.206%
8	8.075	1014	1018	1021	rBV	1140866	845172	16.01%	2.568%
9	8.175	1031	1035	1038	rBV	1584142	1298136	24.59%	3.944%
10	8.298	1053	1056	1058	rVB	92086	64484	1.22%	0.196%
11	8.692	1120	1123	1127	rVB	92034	72021	1.36%	0.219%
12	9.063	1183	1186	1189	rVB	83017	60820	1.15%	0.185%
13	9.251	1213	1218	1222	rBV	5375725	5279145	100.00%	16.038%
14	9.933	1329	1334	1337	rVB	1712725	1432159	27.13%	4.351%
15	10.563	1438	1441	1443	rBV	89042	71955	1.36%	0.219%
16	10.716	1463	1467	1471	rBV	2934758	2770852	52.49%	8.418%
17	10.827	1478	1486	1489	rBV	1191386	1499411	28.40%	4.555%
18	11.416	1582	1586	1590	rBV	1542808	1256918	23.81%	3.818%
19	11.810	1650	1653	1657	rVB	90268	75923	1.44%	0.231%
20	11.939	1671	1675	1680	rBV	196992	193858	3.67%	0.589%
21	12.727	1806	1809	1816	rBV2	125184	125964	2.39%	0.383%
22	13.004	1852	1856	1859	rBV	4673106	4270888	80.90%	12.975%
23	13.851	1997	2000	2003	rBV	55124	68544	1.30%	0.208%
24	13.898	2003	2008	2010	rVV2	289273	289269	5.48%	0.879%
25	13.921	2010	2012	2016	rVB	133558	114220	2.16%	0.347%
26	14.051	2030	2034	2038	rBV	1123677	967439	18.33%	2.939%
27	15.533	2281	2286	2291	rBV	931130	1106696	20.96%	3.362%

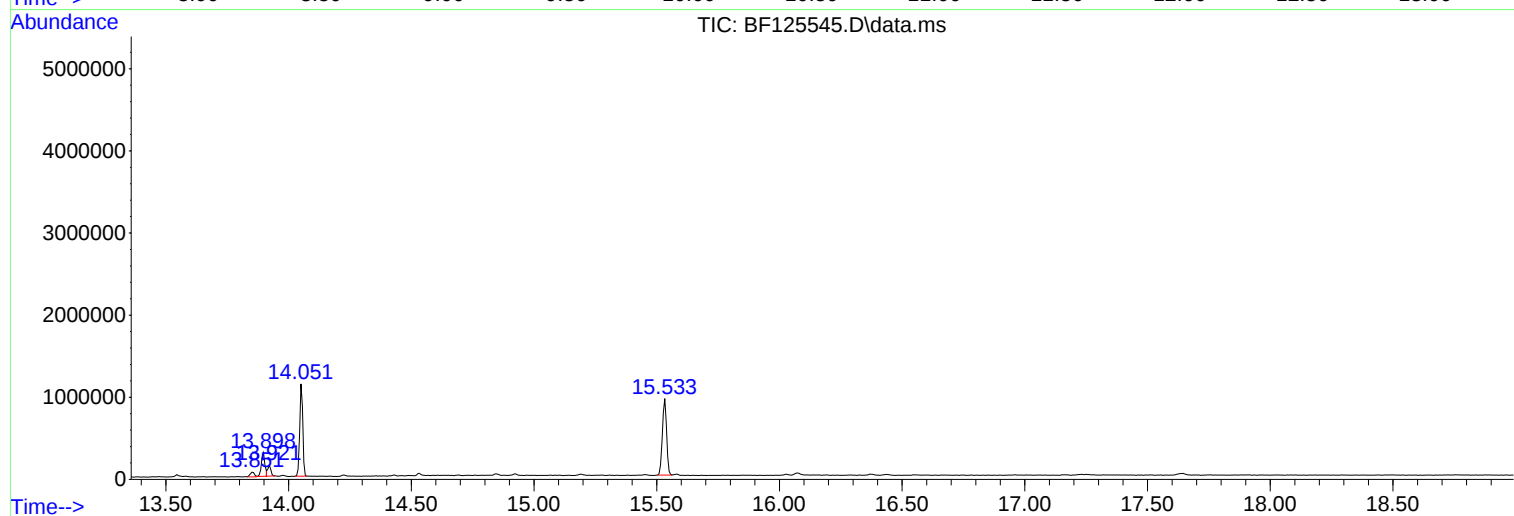
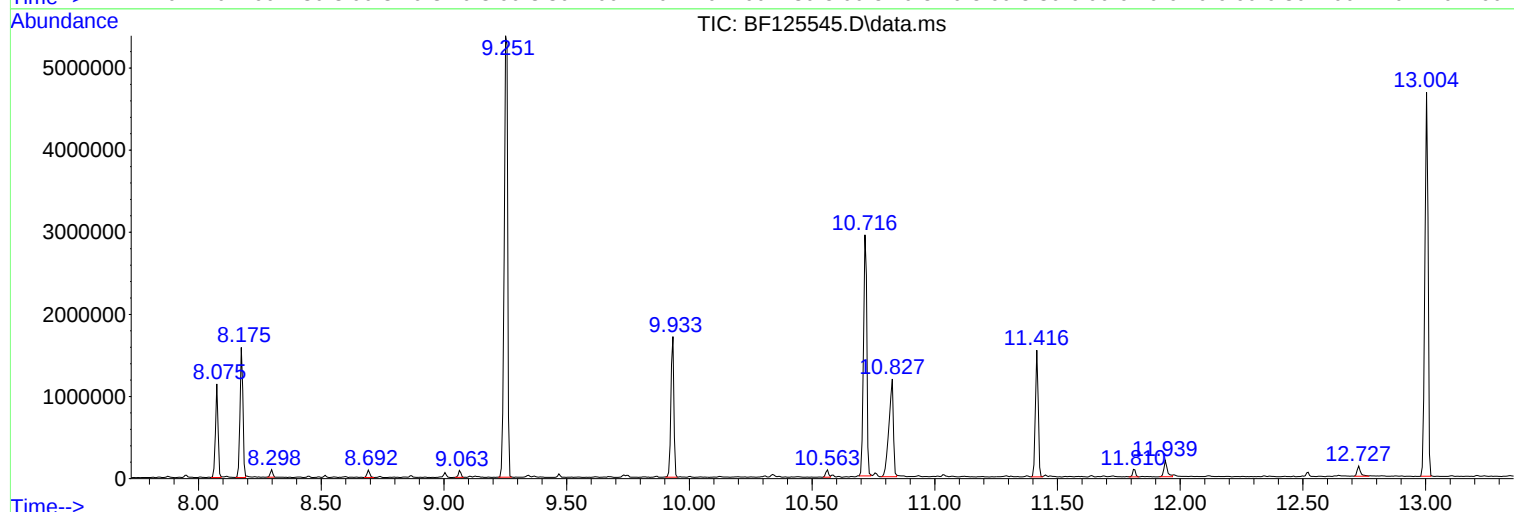
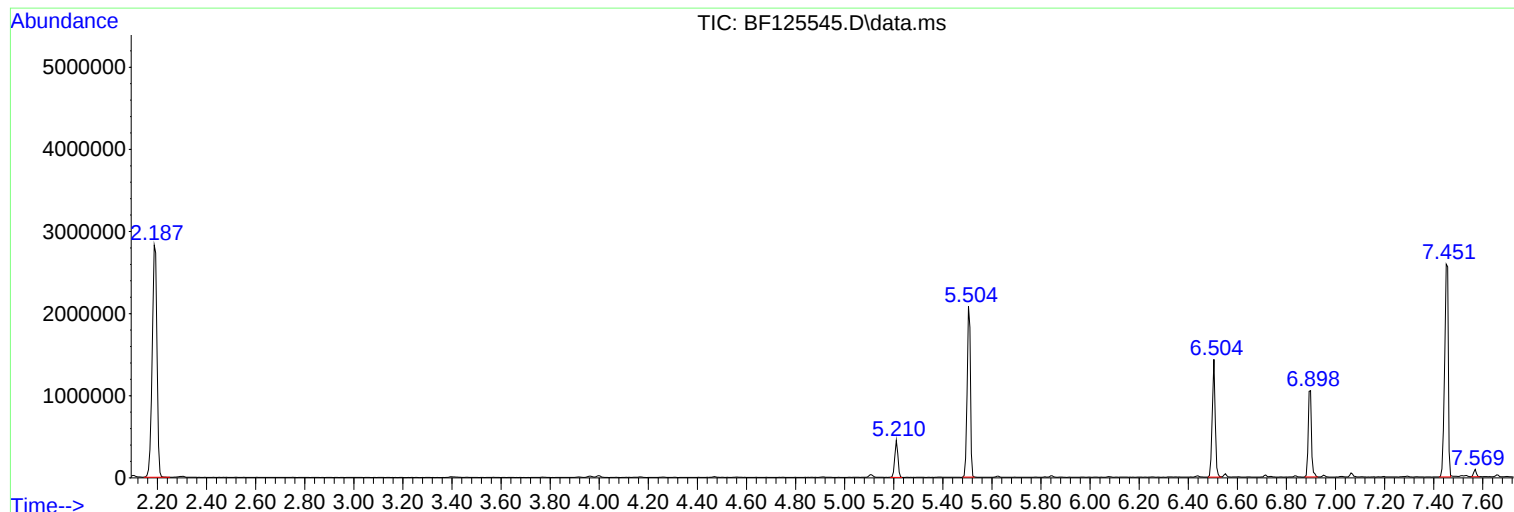
Sum of corrected areas: 32916732

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125545.D
Acq On : 21 Sep 2021 20:12
Operator : JU/CG
Sample : M3835-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-03-(1.0)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.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\BF092121\
Data File : BF125545.D
Acq On : 21 Sep 2021 20:12
Operator : JU/CG
Sample : M3835-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-03-(1.0)

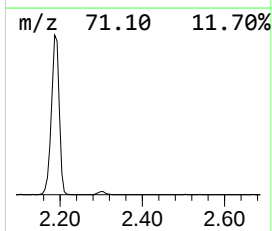
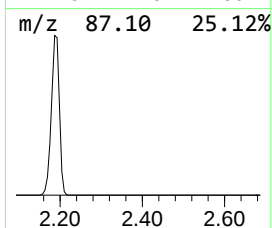
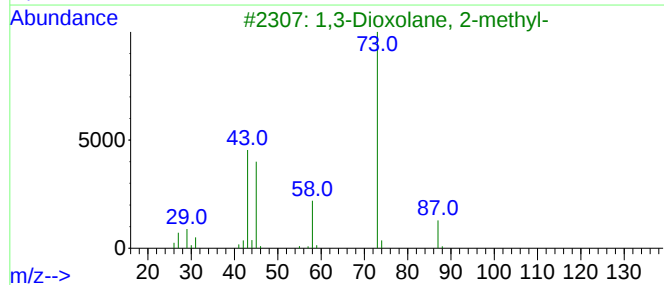
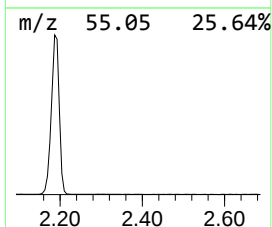
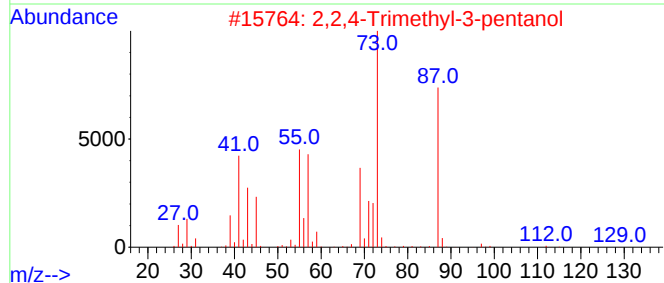
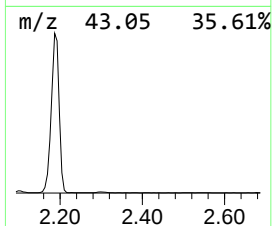
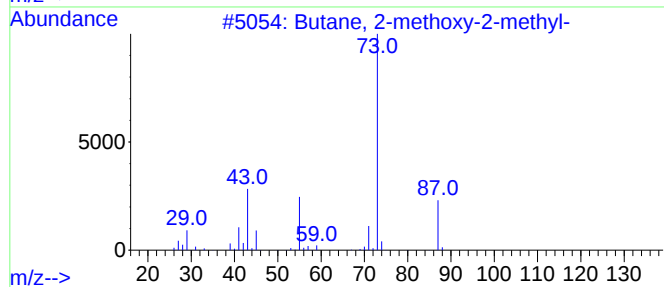
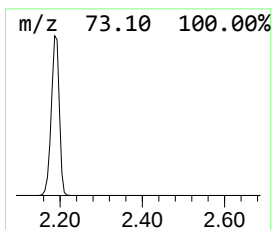
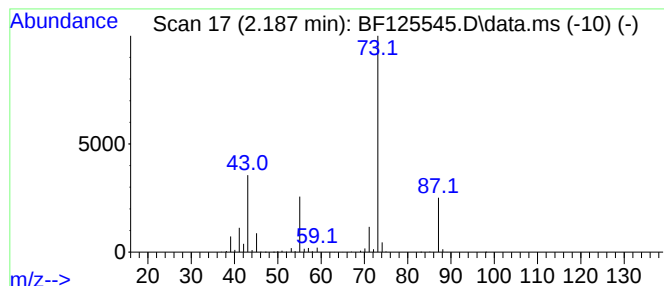
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.187	78.35 ng	3814550	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125545.D
Acq On : 21 Sep 2021 20:12
Operator : JU/CG
Sample : M3835-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-03-(1.0)

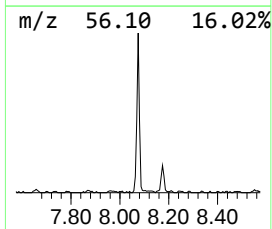
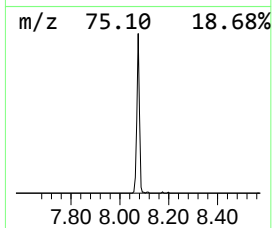
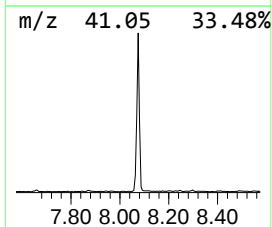
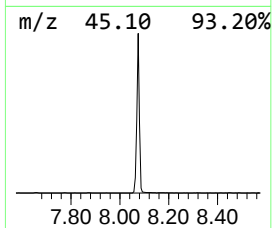
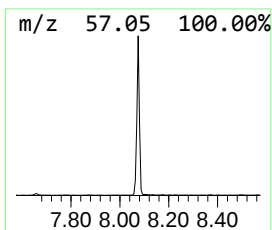
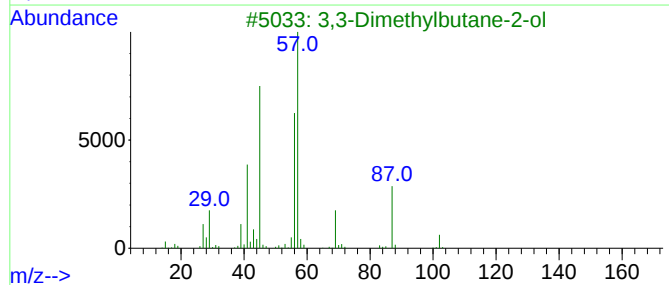
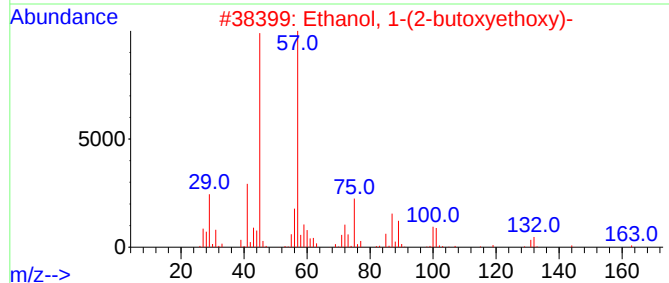
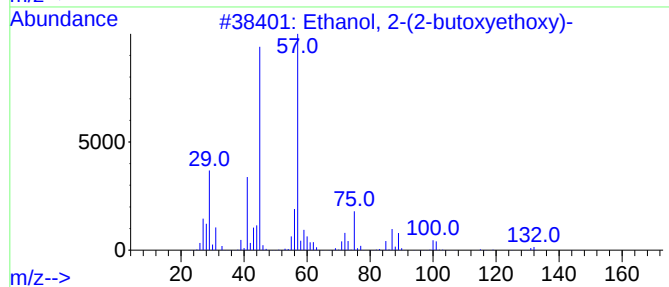
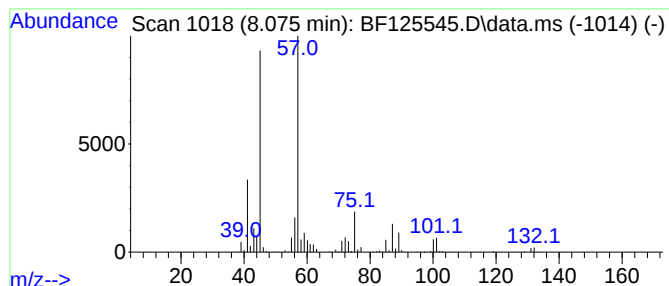
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	13.02 ng	845172	Naphthalene-d8	8.175

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	90
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	58
4			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	53
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125545.D
Acq On : 21 Sep 2021 20:12
Operator : JU/CG
Sample : M3835-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-03-(1.0)

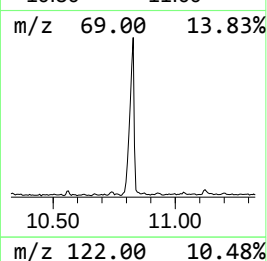
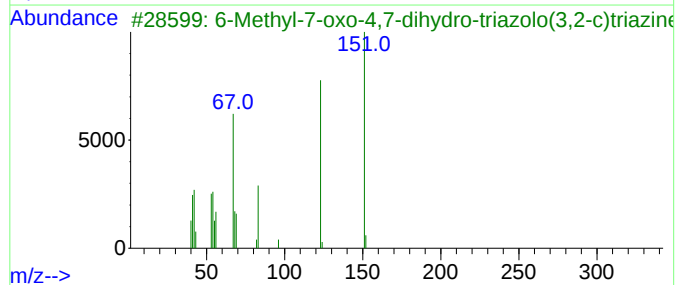
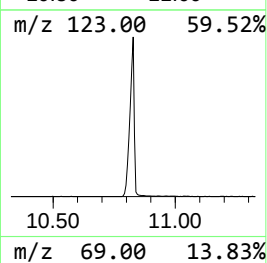
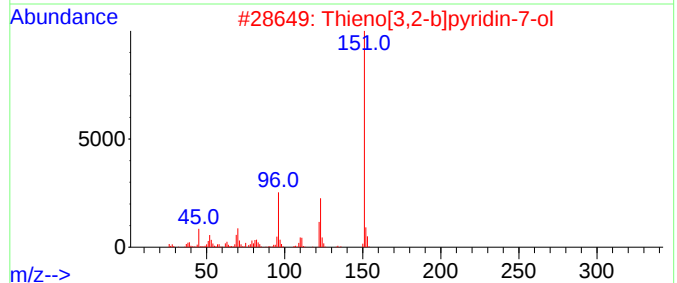
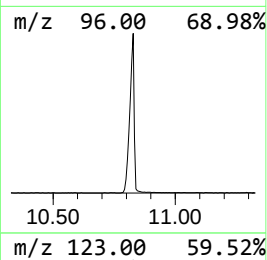
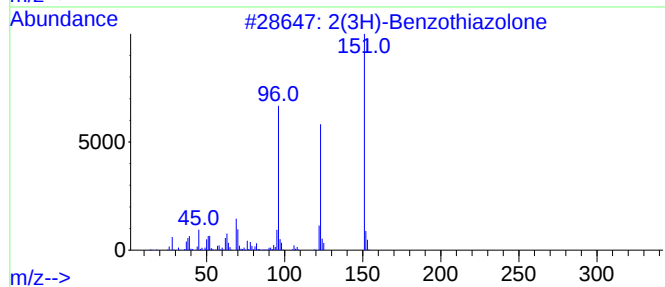
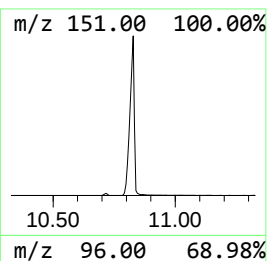
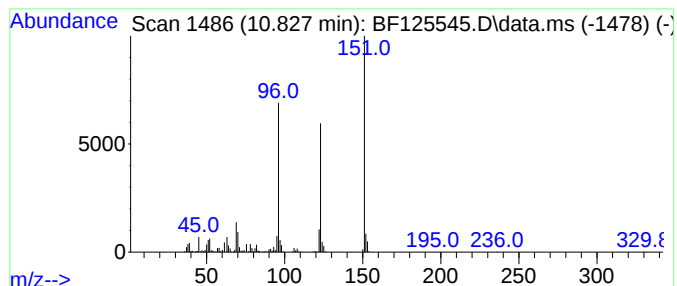
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2(3H)-Benzothiazolone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.827	23.86 ng	1499410	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	97
2			Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	58
3			6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50
4			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	47
5			4-Mercaptoimidazo[4,5-c]pyridine	151	C6H5N3S	034550-51-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125545.D
Acq On : 21 Sep 2021 20:12
Operator : JU/CG
Sample : M3835-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-03-(1.0)

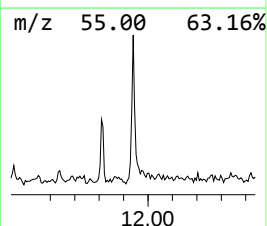
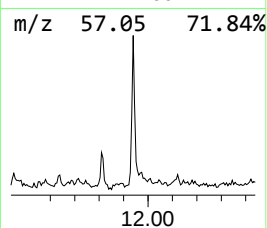
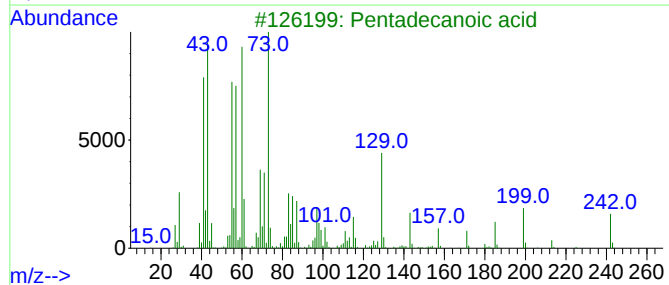
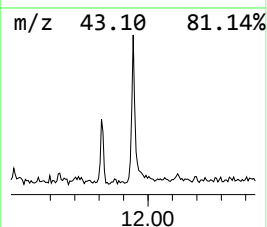
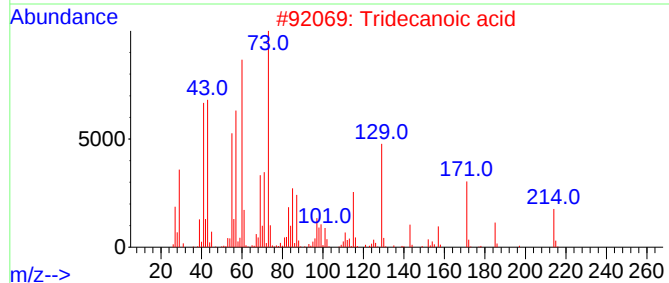
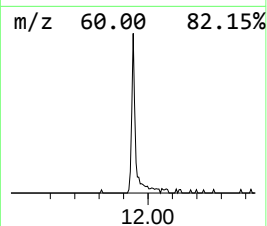
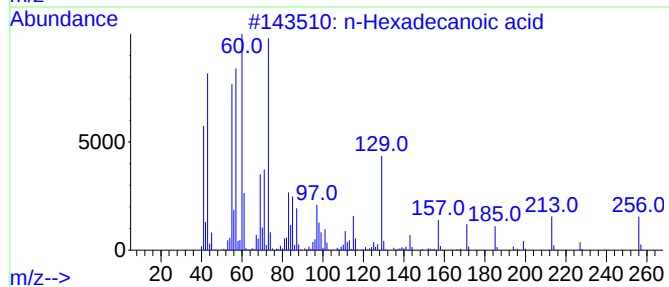
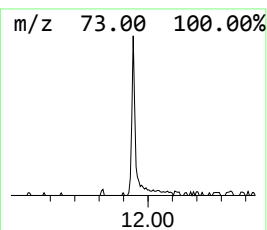
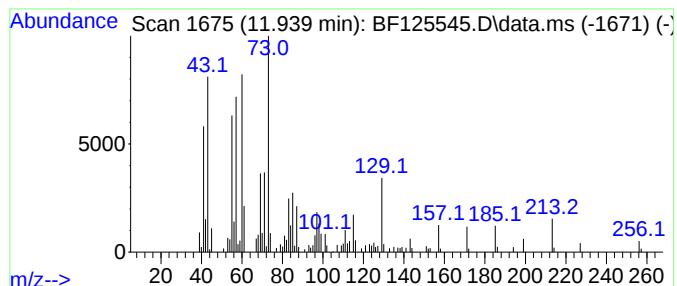
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	3.08 ng	193858	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125545.D
Acq On : 21 Sep 2021 20:12
Operator : JU/CG
Sample : M3835-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-03-(1.0)

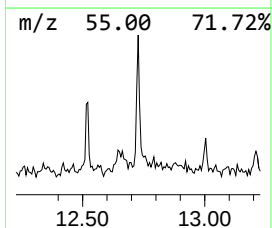
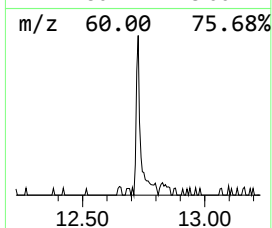
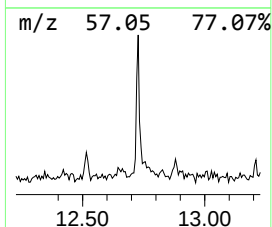
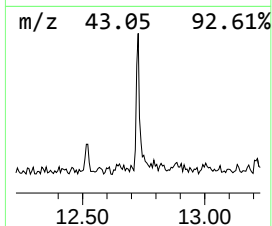
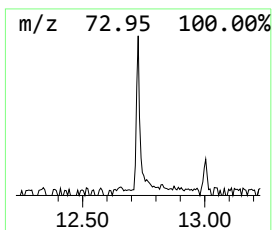
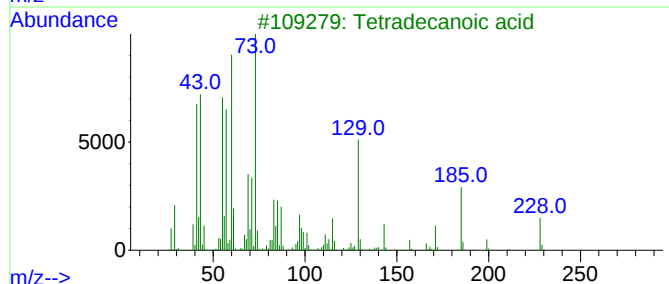
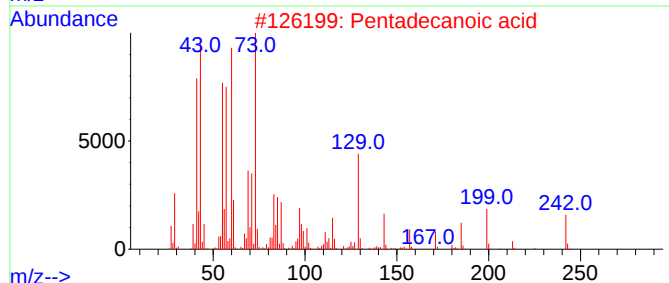
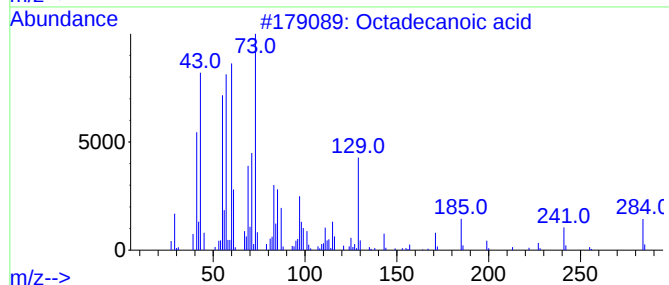
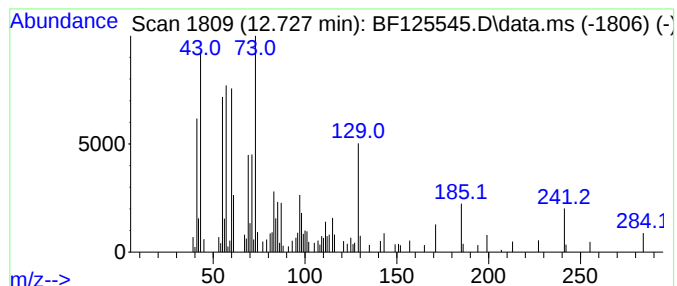
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	2.00 ng	125964	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
5			n-Decanoic acid	172	C10H20O2	000334-48-5	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125545.D
Acq On : 21 Sep 2021 20:12
Operator : JU/CG
Sample : M3835-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

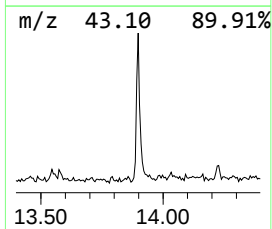
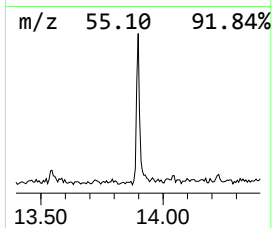
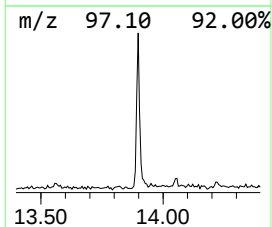
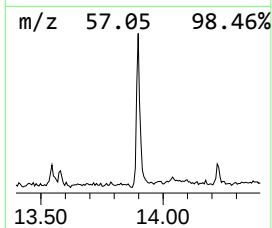
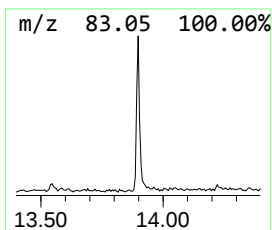
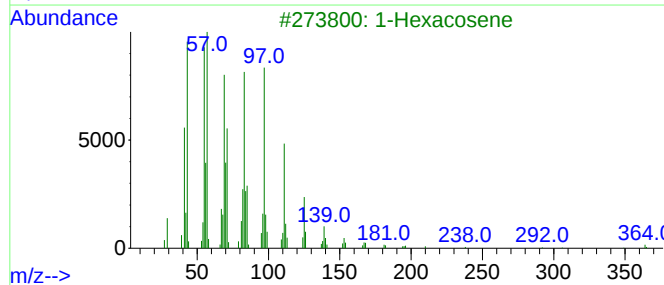
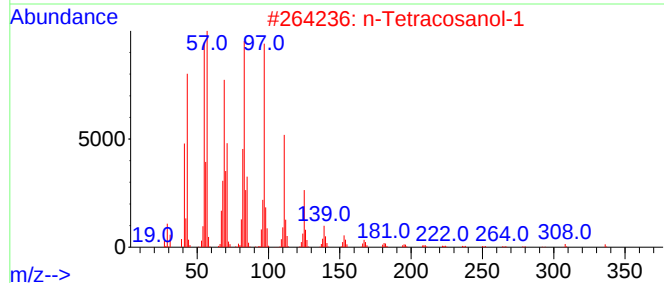
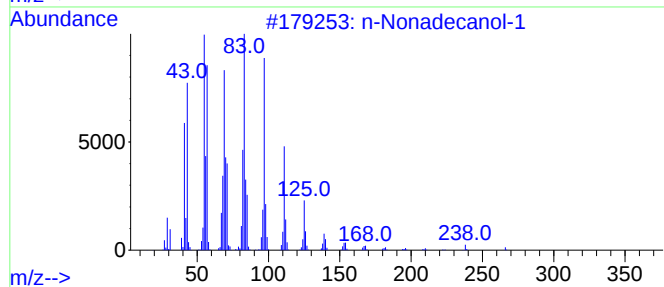
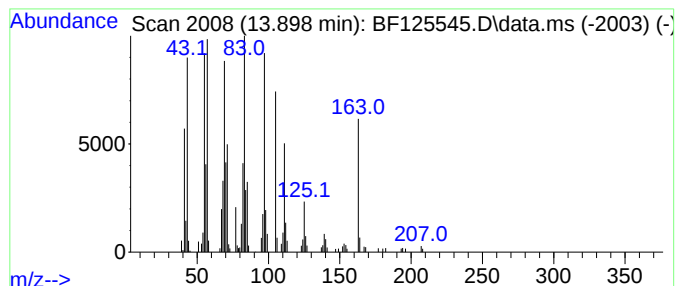
Instrument :
BNA_F
ClientSampleId :
SW-CB-03-(1.0)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.898	5.98 ng	289269	Chrysene-d12	14.051	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	1-Hexacosene	364	C26H52	018835-33-1	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125545.D
Acq On : 21 Sep 2021 20:12
Operator : JU/CG
Sample : M3835-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-03-(1.0)

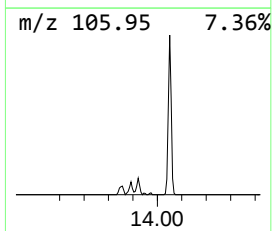
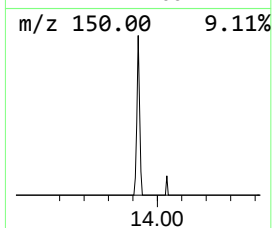
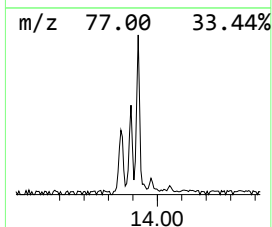
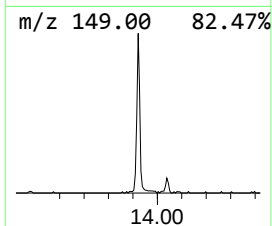
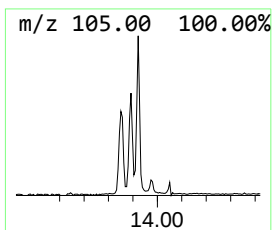
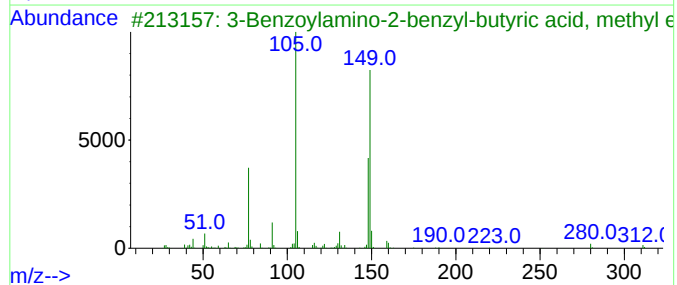
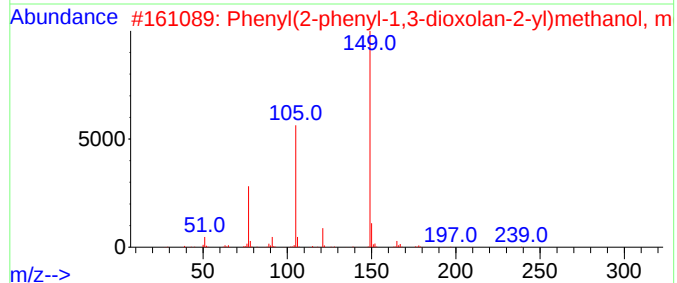
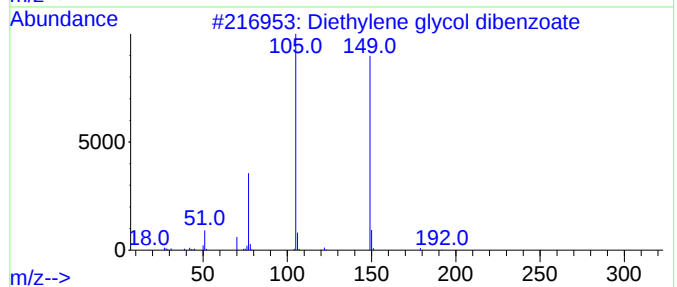
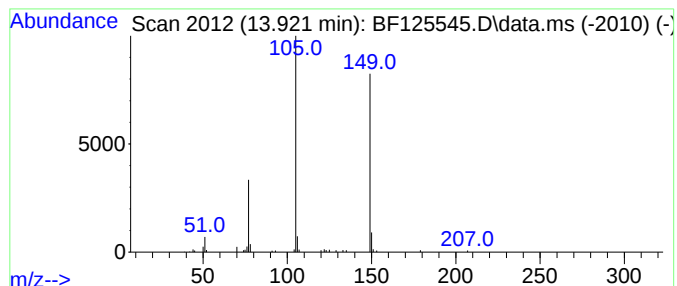
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	2.36 ng	114220	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2			Phenyl(2-phenyl-1,3-dioxolan-2-yl)methanol	270	C17H18O3	1000507-07-6	78
3			3-Benzoylamino-2-benzyl-butyric acid	311	C19H21NO3	1000193-12-7	78
4			2,2'-(Ethane-1,2-diylbis(oxy))bis(phenyl)	358	C20H22O6	1000366-99-4	78
5			Benzoic acid, 2-(4-nitrophenoxy)	287	C15H13NO5	1000368-92-7	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125545.D
Acq On : 21 Sep 2021 20:12
Operator : JU/CG
Sample : M3835-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-03-(1.0)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.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
Butane, 2-metho...	2.187	78.3	ng	3814550	1	6.898	973768	20.0
Ethanol, 2-(2-b...	8.075	13.0	ng	845172	2	8.175	1298140	20.0
2(3H)-Benzothia...	10.827	23.9	ng	1499410	4	11.416	1256920	20.0
n-Hexadecanoic ...	11.939	3.1	ng	193858	4	11.416	1256920	20.0
Octadecanoic acid	12.727	2.0	ng	125964	4	11.416	1256920	20.0
n-Nonadecanol-1	13.898	6.0	ng	289269	5	14.051	967439	20.0
Diethylene glyc...	13.921	2.4	ng	114220	5	14.051	967439	20.0