

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
 Data File : BF125211.D
 Acq On : 25 Aug 2021 15:52
 Operator : JU/CG
 Sample : M3524-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-1

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125211.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	14	21	27	rVB	923293	1204029	32.20%	4.581%
2	5.534	581	586	589	rBV	3472394	3362931	89.94%	12.794%
3	6.534	751	756	759	rBV	3219823	3367330	90.06%	12.811%
4	6.910	817	820	824	rBV	951342	852318	22.80%	3.243%
5	7.475	911	916	919	rBV	2547060	2223401	59.47%	8.459%
6	8.092	1018	1021	1035	rBV	107043	206217	5.52%	0.785%
7	8.198	1035	1039	1042	rVV	1239175	1088282	29.11%	4.140%
8	9.269	1217	1221	1224	rBV	4424247	3738885	100.00%	14.225%
9	9.951	1333	1337	1340	rBV	1420514	1167967	31.24%	4.444%
10	10.739	1467	1471	1474	rBV	2734696	2337842	62.53%	8.894%
11	11.439	1586	1590	1593	rBV	1173779	1107702	29.63%	4.214%
12	11.951	1673	1677	1682	rBV	177574	185168	4.95%	0.704%
13	12.739	1807	1811	1819	rBV	75936	88909	2.38%	0.338%
14	13.021	1855	1859	1862	rBV	3827055	3211033	85.88%	12.216%
15	13.910	2006	2010	2013	rBV	39833	43786	1.17%	0.167%
16	13.945	2013	2016	2019	rVV	89049	89583	2.40%	0.341%
17	13.992	2019	2024	2033	rVV	37000	127747	3.42%	0.486%
18	14.074	2035	2038	2042	rVB	941489	837437	22.40%	3.186%
19	15.574	2287	2293	2300	rBV	766994	1001211	26.78%	3.809%
20	16.051	2370	2374	2379	rVB2	28408	43011	1.15%	0.164%

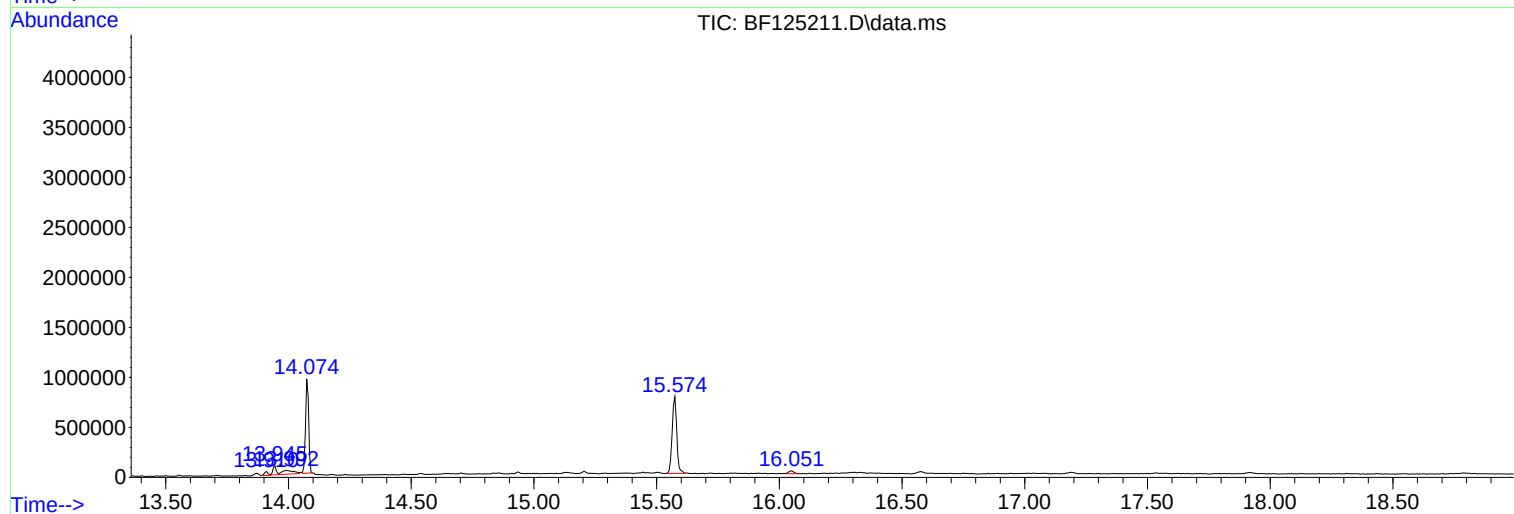
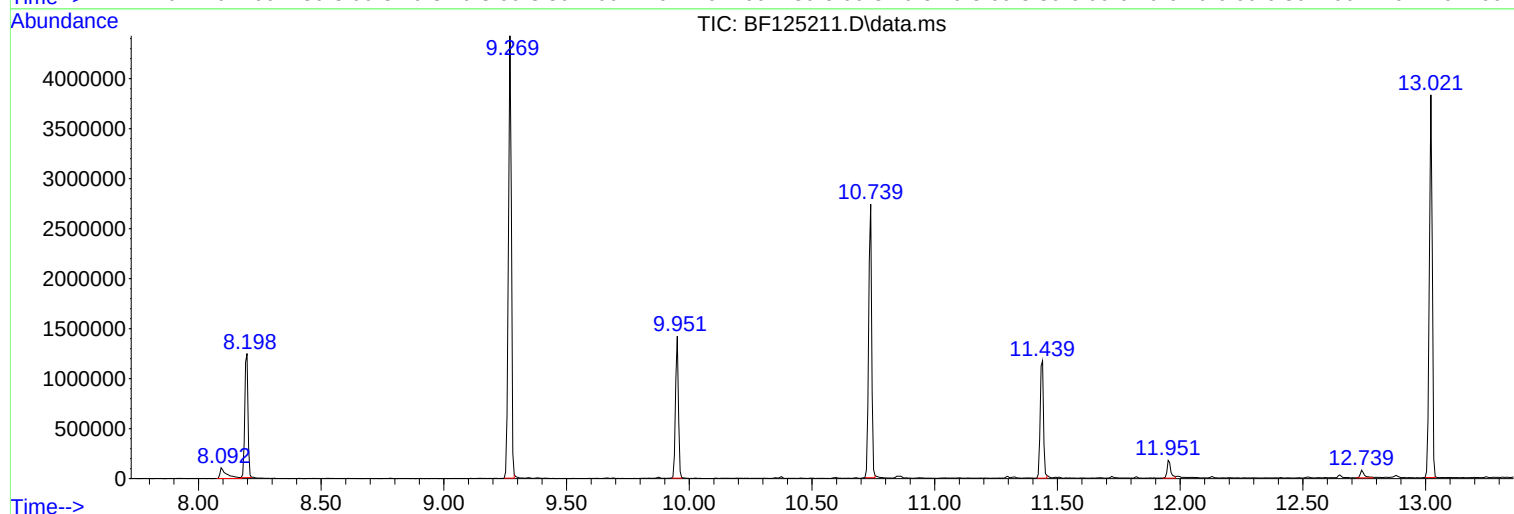
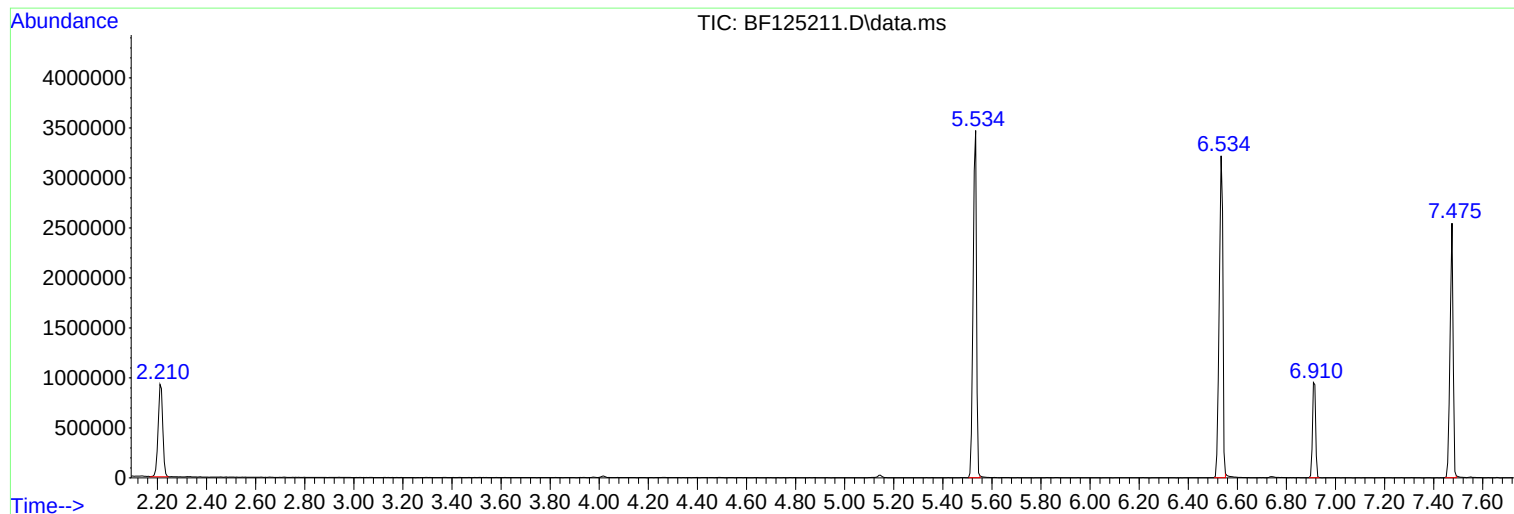
Sum of corrected areas: 26284789

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125211.D
Acq On : 25 Aug 2021 15:52
Operator : JU/CG
Sample : M3524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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\BF082521\
Data File : BF125211.D
Acq On : 25 Aug 2021 15:52
Operator : JU/CG
Sample : M3524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-1

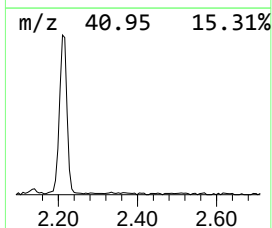
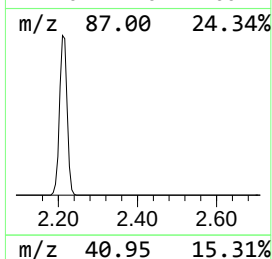
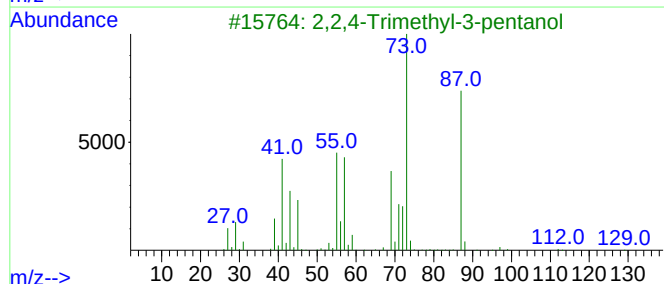
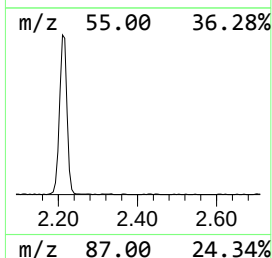
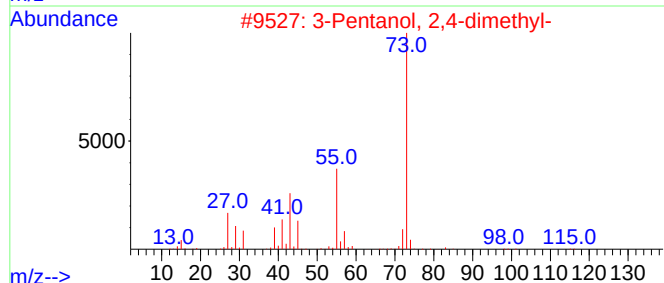
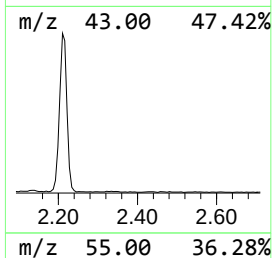
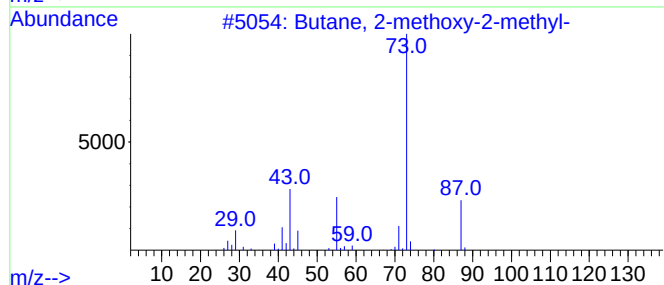
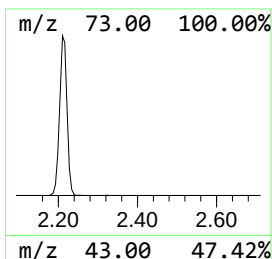
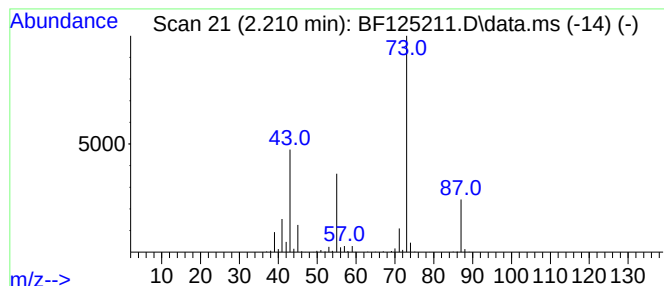
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.210	28.25 ng	1204030	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125211.D
Acq On : 25 Aug 2021 15:52
Operator : JU/CG
Sample : M3524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-1

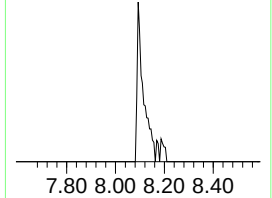
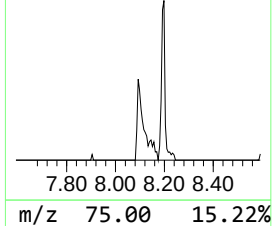
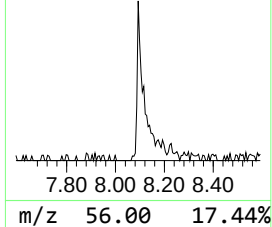
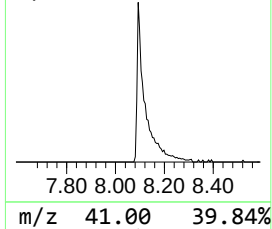
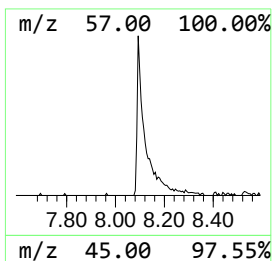
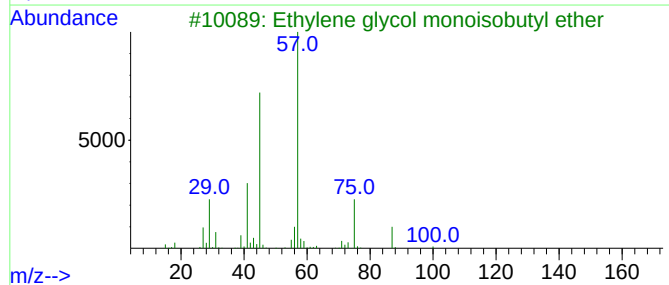
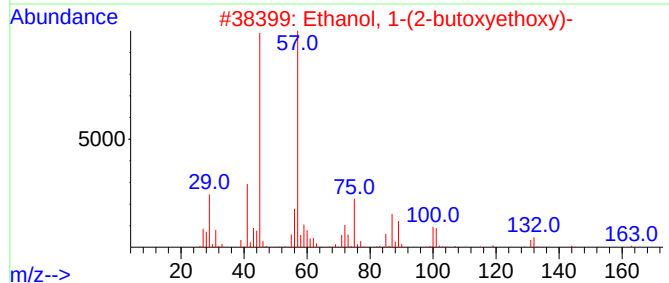
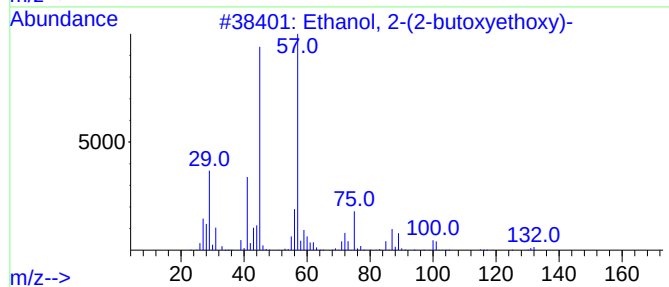
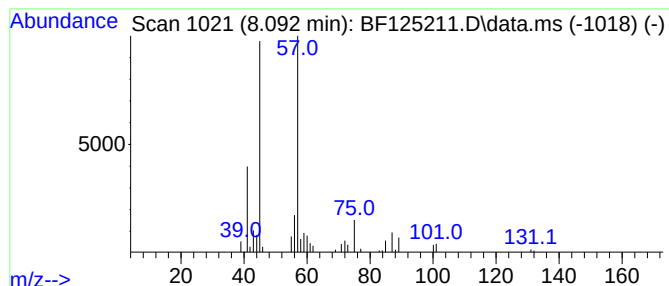
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	3.79 ng	206217	Naphthalene-d8	8.198

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	78
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125211.D
Acq On : 25 Aug 2021 15:52
Operator : JU/CG
Sample : M3524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-1

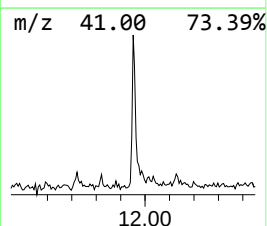
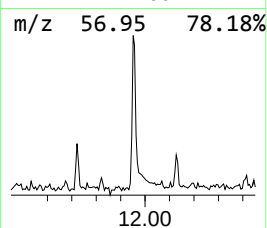
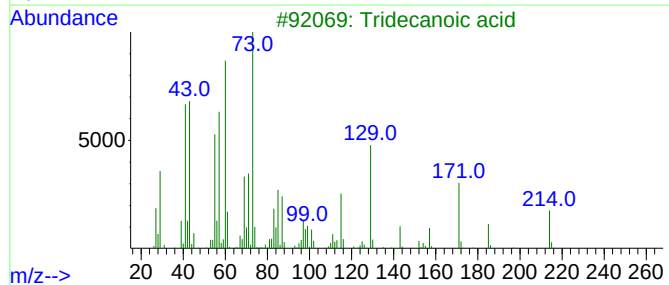
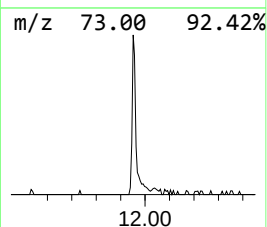
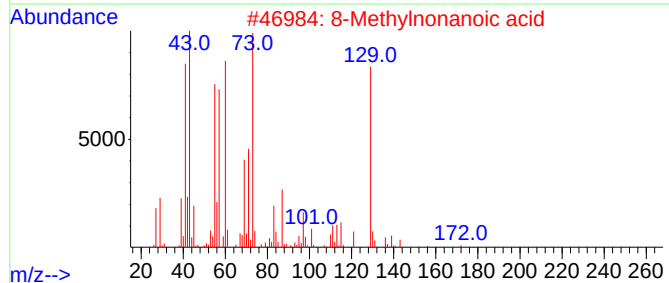
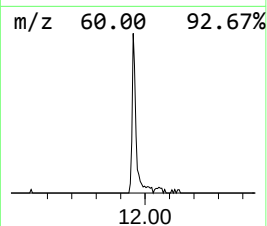
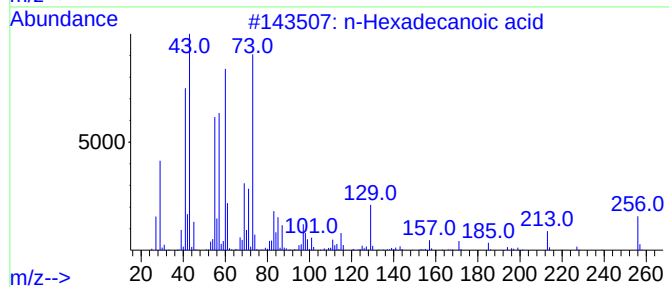
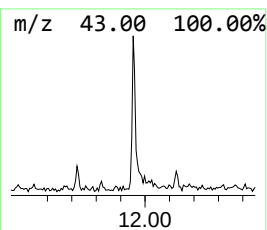
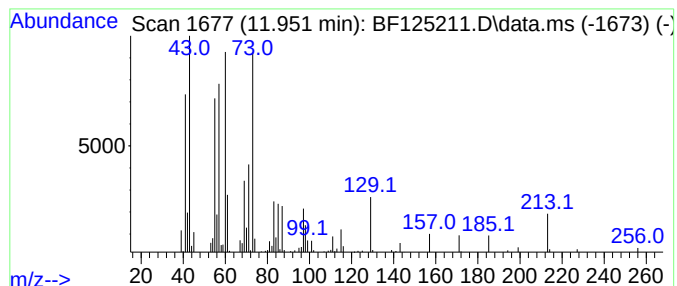
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.951	3.34 ng	185168	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
2			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5			Isoamyl nitrite	117	C5H11NO2	000110-46-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125211.D
Acq On : 25 Aug 2021 15:52
Operator : JU/CG
Sample : M3524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-1

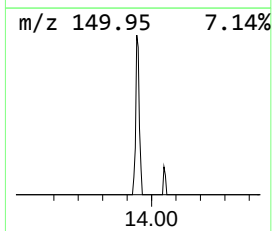
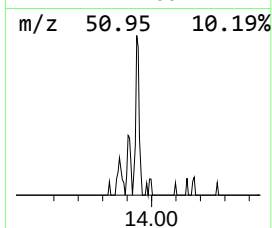
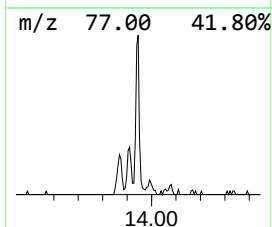
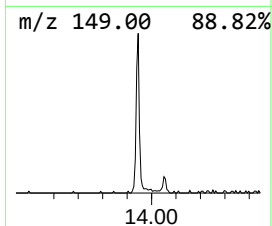
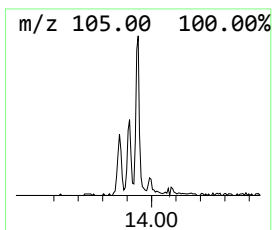
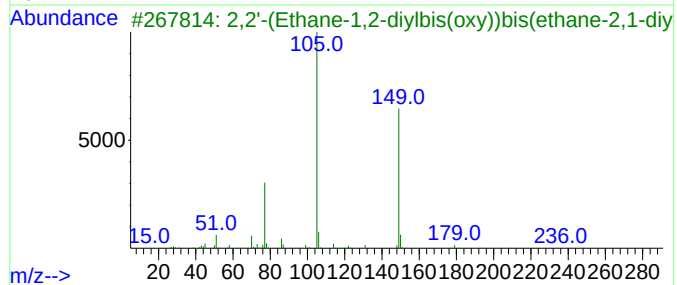
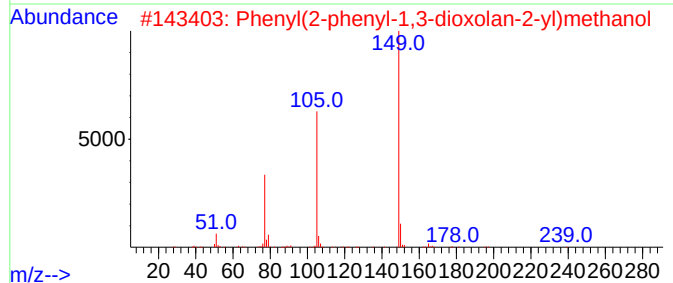
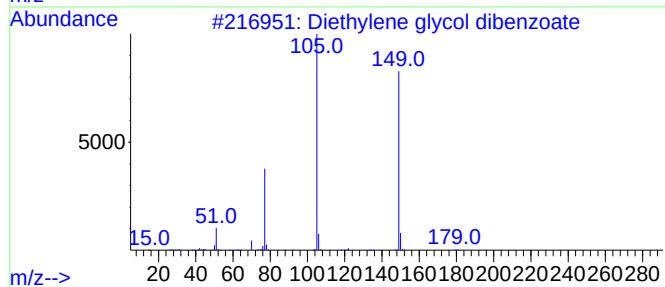
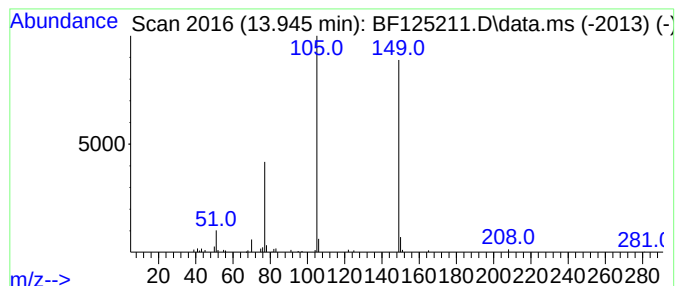
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	2.14 ng	89583	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
2			Phenyl(2-phenyl-1,3-dioxolan-2-yl)methanol	256	C16H16O3	005694-69-9	78
3			2,2'-(Ethane-1,2-diylbis(oxy))bis(ethane-2,1-diyl)	358	C20H22O6	1000366-99-4	78
4			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
5			Benzoic acid N'-(4,4,5,5,6,6-hexafluoro-1,3-dioxane-2-yl)methanol	434	C19H13F7NO2	1000295-76-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125211.D
Acq On : 25 Aug 2021 15:52
Operator : JU/CG
Sample : M3524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-1

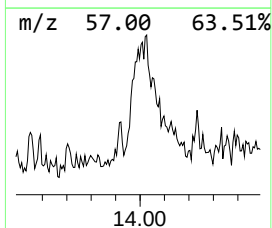
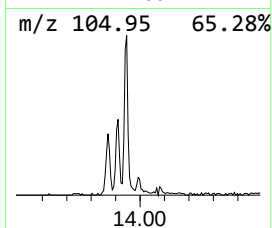
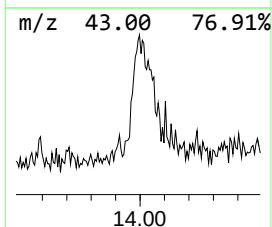
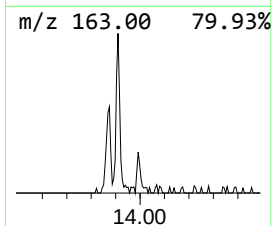
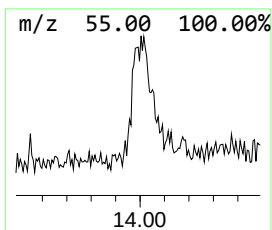
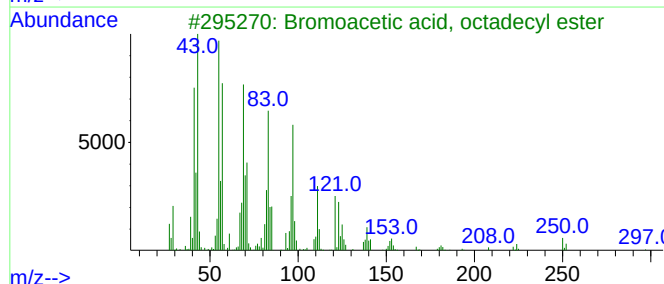
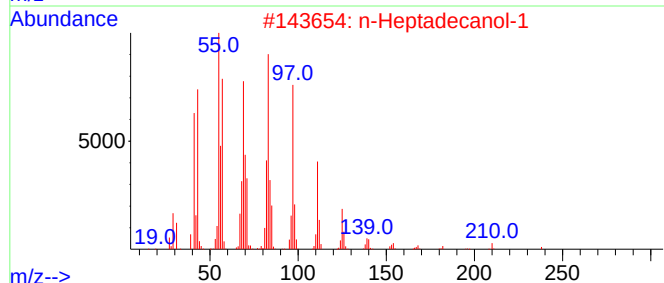
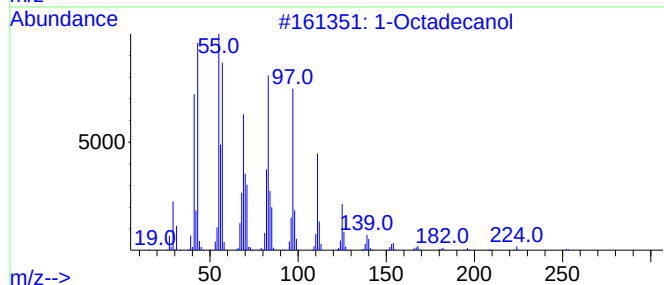
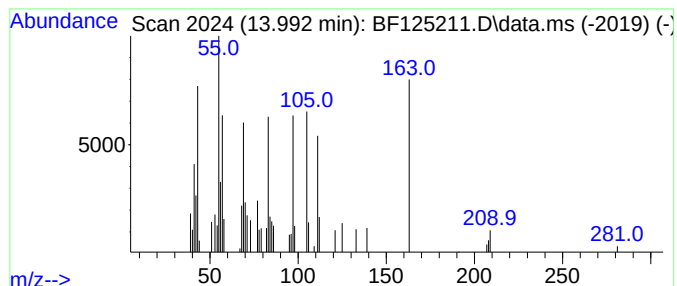
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.992 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	3.05 ng	127747	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanol	270	C18H38O	000112-92-5	42
2			n-Heptadecanol-1	256	C17H36O	001454-85-9	38
3			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	35
4			1-Tetracosene	336	C24H48	010192-32-2	27
5			1-Heptacosanol	396	C27H56O	002004-39-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125211.D
Acq On : 25 Aug 2021 15:52
Operator : JU/CG
Sample : M3524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.210	28.3	ng	1204030	1	6.916	852318	20.0
Ethanol, 2-(2-b...	8.092	3.8	ng	206217	2	8.198	1088280	20.0
n-Hexadecanoic ...	11.951	3.3	ng	185168	4	11.439	1107700	20.0
Diethylene glyc...	13.945	2.1	ng	89583	5	14.074	837437	20.0
unknown13.992	13.992	3.0	ng	127747	5	14.074	837437	20.0