

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
 Data File : BF125115.D
 Acq On : 19 Aug 2021 15:33
 Operator : JU/CG
 Sample : M3449-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP2

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: BF125115.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	18	25	33	rVB	1501167	1999095	46.46%	5.453%
2	5.151	513	521	527	rVB	140925	173197	4.02%	0.472%
3	5.534	581	586	589	rBV	3872612	4140973	96.23%	11.295%
4	6.534	751	756	759	rBV	3562441	4201888	97.64%	11.461%
5	6.916	818	821	825	rVB	1343051	1112559	25.85%	3.035%
6	7.481	912	917	920	rBV	2954239	2782275	64.65%	7.589%
7	8.098	1018	1022	1028	rBV	881972	748081	17.38%	2.040%
8	8.198	1035	1039	1043	rBV	1692514	1483570	34.48%	4.046%
9	9.275	1217	1222	1226	rBV	4412924	4303290	100.00%	11.737%
10	9.957	1334	1338	1341	rBV	2024642	1649741	38.34%	4.500%
11	10.745	1467	1472	1475	rBV	3389780	3018110	70.13%	8.232%
12	11.445	1587	1591	1593	rBV	2067655	1737963	40.39%	4.740%
13	11.469	1593	1595	1597	rVB	179764	140791	3.27%	0.384%
14	11.833	1654	1657	1659	rBV	77759	55488	1.29%	0.151%
15	11.963	1673	1679	1687	rBV3	327097	411860	9.57%	1.123%
16	12.051	1691	1694	1697	rBV2	56957	58226	1.35%	0.159%
17	12.492	1763	1769	1772	rBV	63005	61811	1.44%	0.169%
18	12.539	1772	1777	1781	rVB3	91623	124401	2.89%	0.339%
19	12.657	1794	1797	1802	rBV	279024	257553	5.99%	0.702%
20	12.751	1810	1813	1817	rBV	126656	143323	3.33%	0.391%
21	12.886	1830	1836	1841	rVB	266173	285503	6.63%	0.779%
22	13.033	1856	1861	1864	rBV	4373440	4025945	93.56%	10.981%
23	13.715	1971	1977	1981	rBV2	44333	55739	1.30%	0.152%
24	13.833	1991	1997	2000	rBV2	32789	50616	1.18%	0.138%
25	13.933	2009	2014	2031	rBV6	135191	458289	10.65%	1.250%
26	14.080	2034	2039	2042	rVV	1319063	1345691	31.27%	3.670%
27	14.104	2042	2043	2050	rVB	132480	121644	2.83%	0.332%
28	14.592	2121	2126	2134	rBV8	62912	160611	3.73%	0.438%
29	15.133	2214	2218	2222	rBV	89249	147265	3.42%	0.402%
30	15.215	2229	2232	2235	rVB	52588	48527	1.13%	0.132%
31	15.445	2268	2271	2278	rVB	56742	70268	1.63%	0.192%
32	15.509	2278	2282	2288	rBV	68461	91147	2.12%	0.249%
33	15.580	2289	2294	2299	rBV	821788	1019988	23.70%	2.782%
34	16.062	2372	2376	2381	rVB3	34183	48156	1.12%	0.131%
35	17.080	2543	2549	2556	rVB2	34819	74332	1.73%	0.203%
36	17.533	2621	2626	2632	rBV2	29902	55438	1.29%	0.151%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125115.D
Acq On : 19 Aug 2021 15:33
Operator : JU/CG
Sample : M3449-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

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

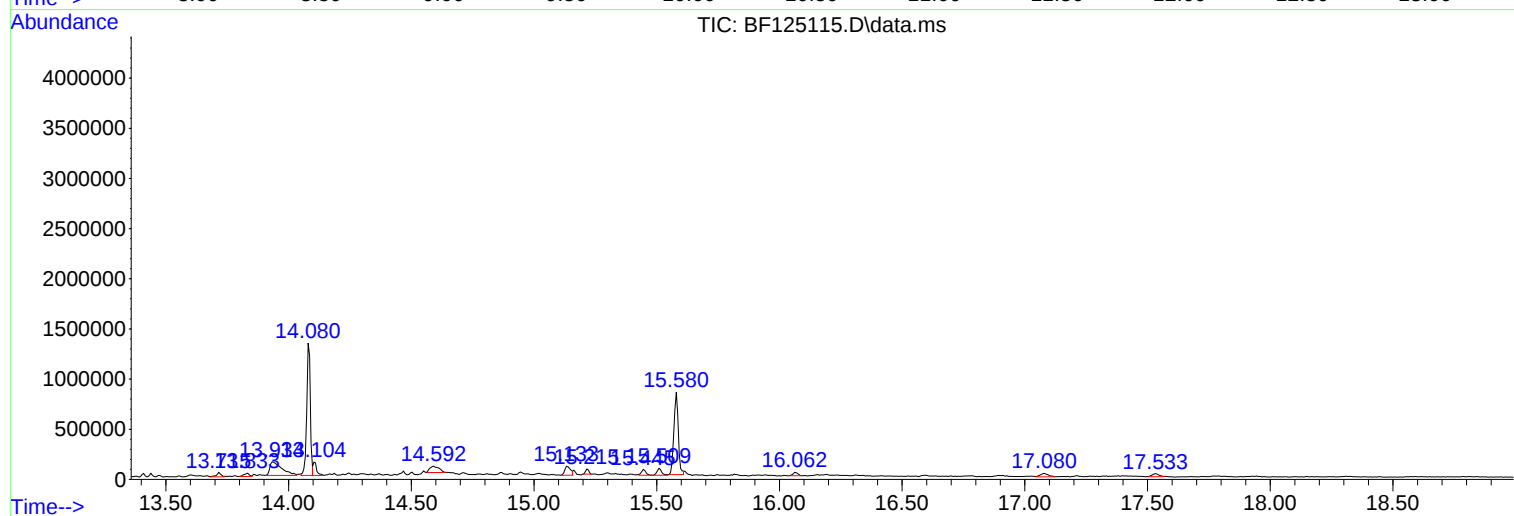
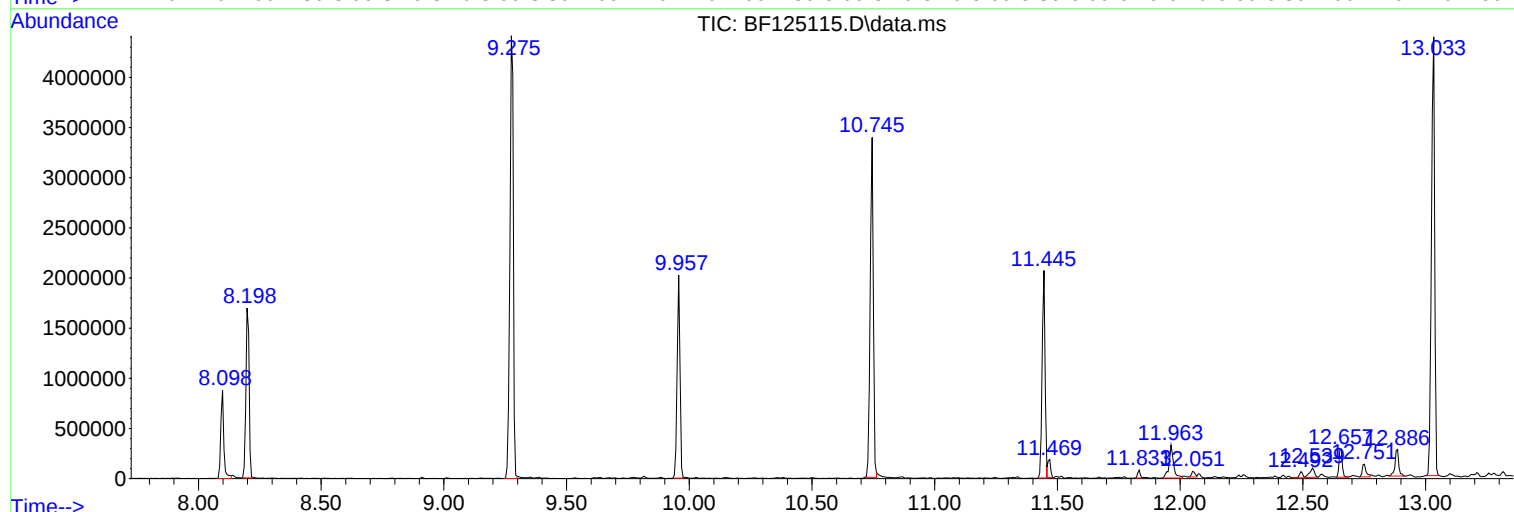
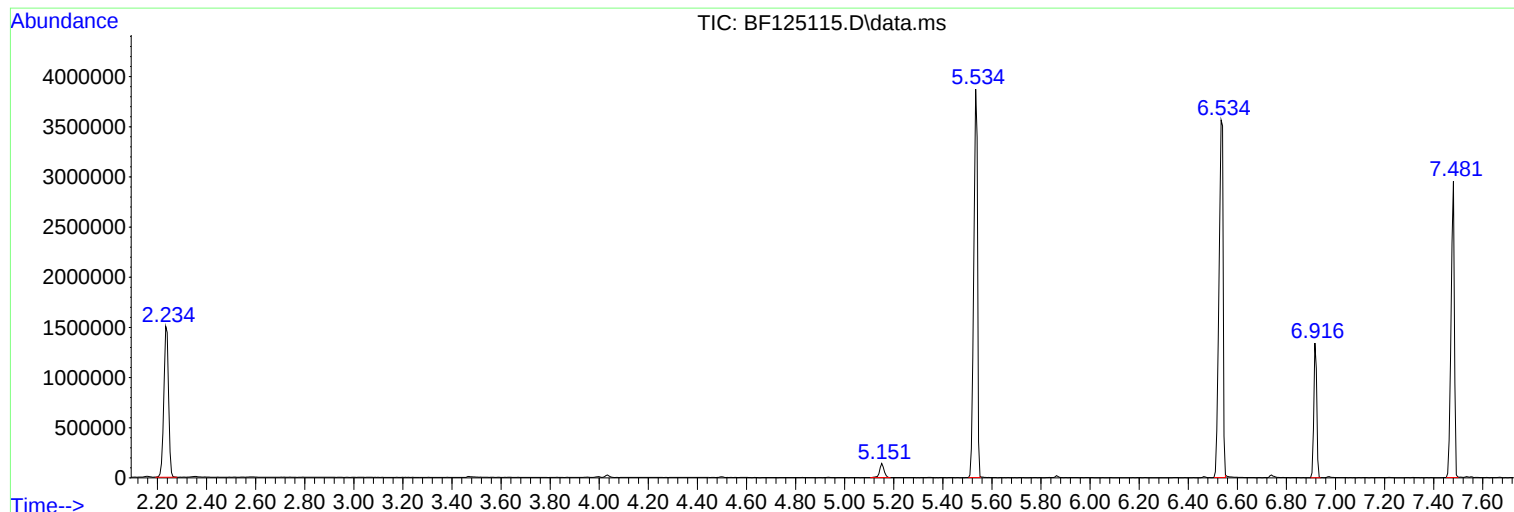
Sum of corrected areas: 36663354

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125115.D
Acq On : 19 Aug 2021 15:33
Operator : JU/CG
Sample : M3449-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

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\BF081921\
Data File : BF125115.D
Acq On : 19 Aug 2021 15:33
Operator : JU/CG
Sample : M3449-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

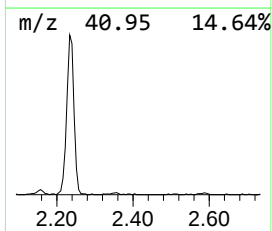
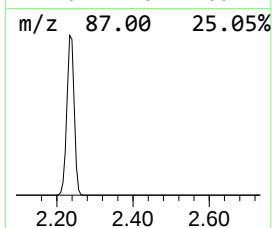
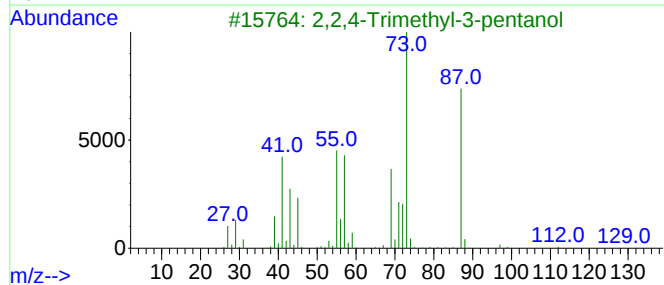
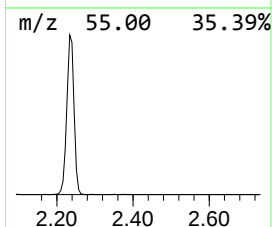
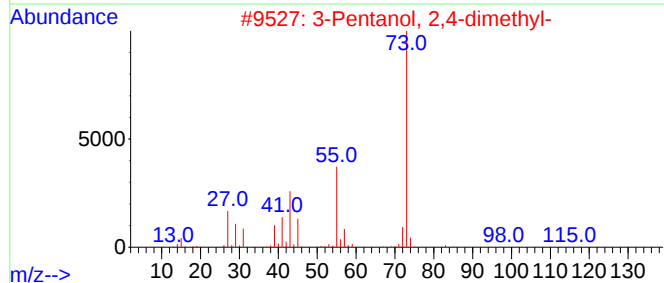
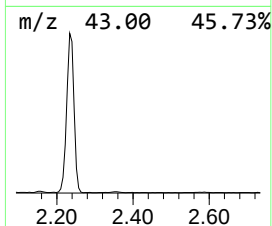
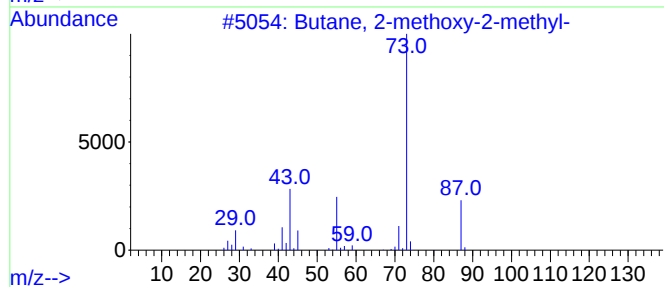
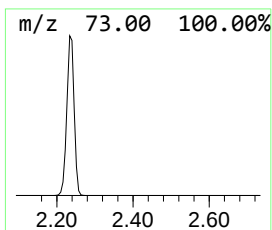
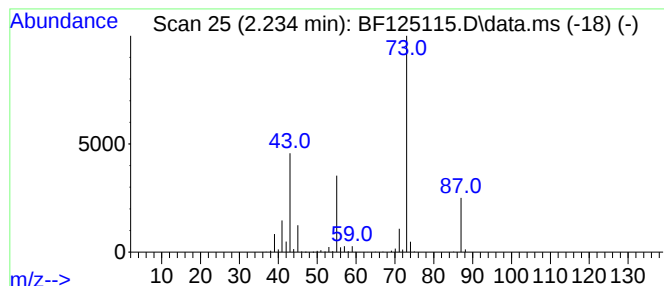
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.234	35.94 ng	1999100	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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125115.D
Acq On : 19 Aug 2021 15:33
Operator : JU/CG
Sample : M3449-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
TP2

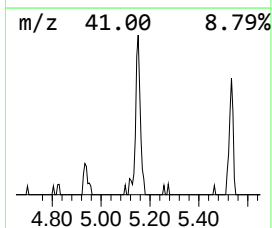
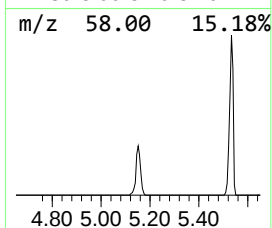
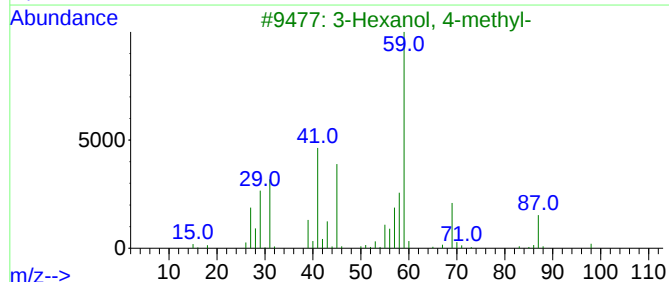
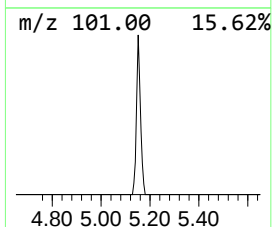
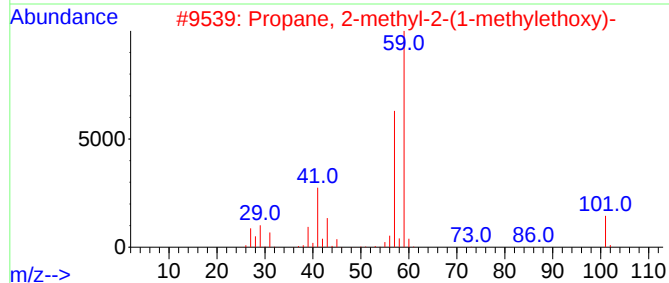
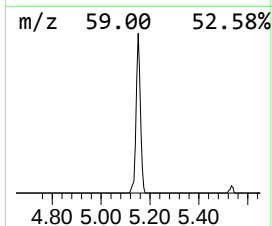
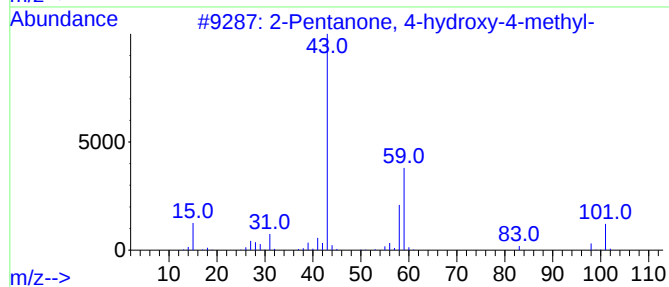
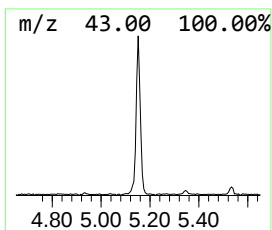
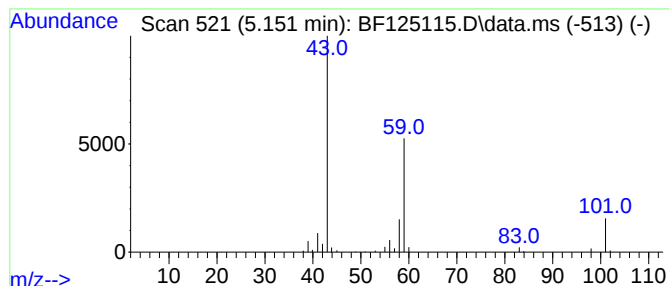
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	3.11 ng	173197	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125115.D
Acq On : 19 Aug 2021 15:33
Operator : JU/CG
Sample : M3449-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

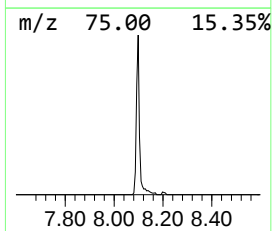
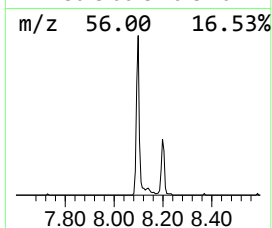
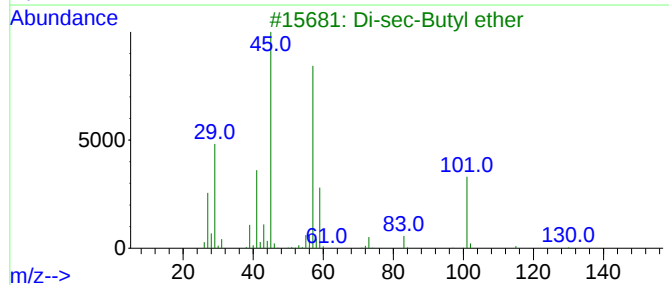
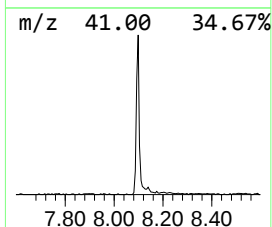
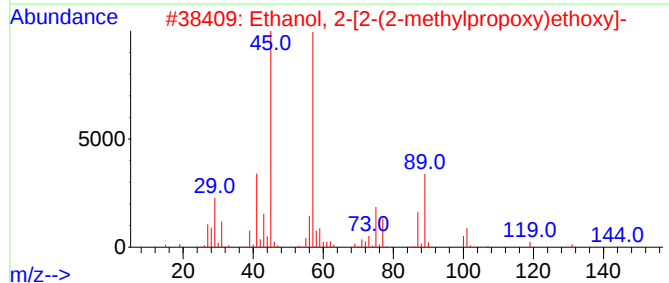
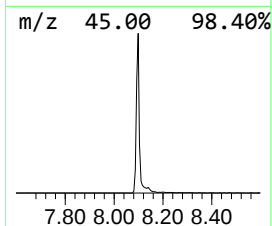
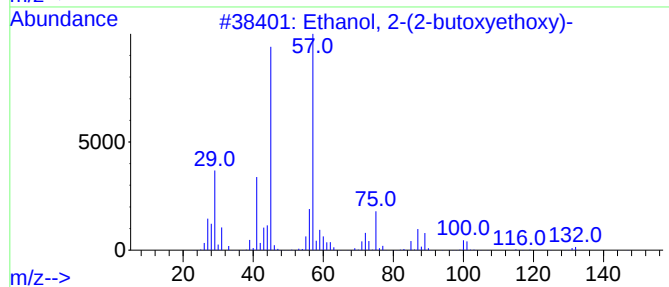
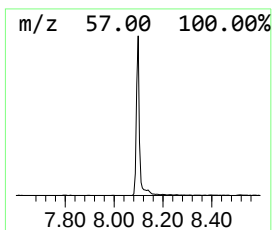
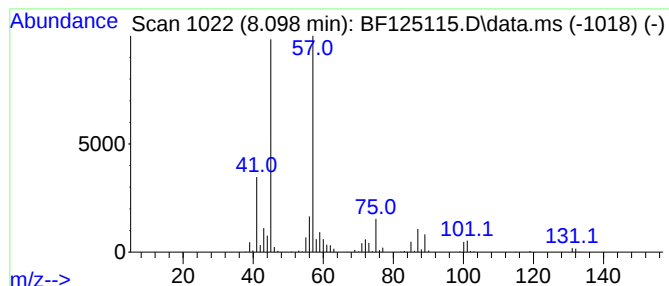
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	10.08 ng	748081	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, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Butyl lactate	146	C7H14O3	000138-22-7	47
5			Paraldehyde	132	C6H12O3	000123-63-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125115.D
Acq On : 19 Aug 2021 15:33
Operator : JU/CG
Sample : M3449-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

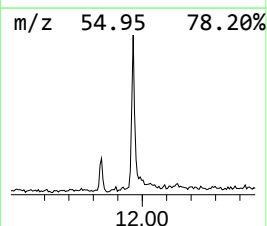
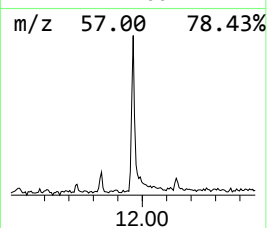
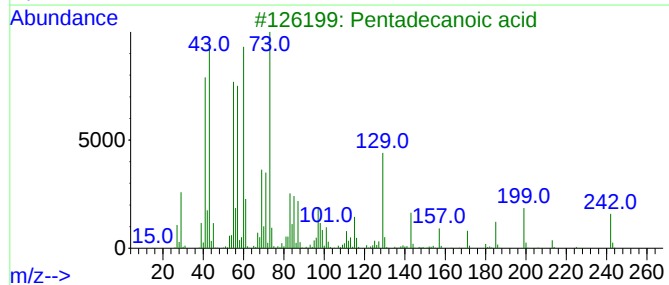
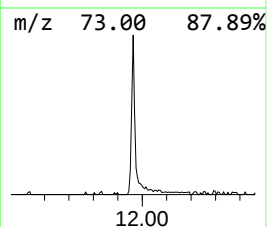
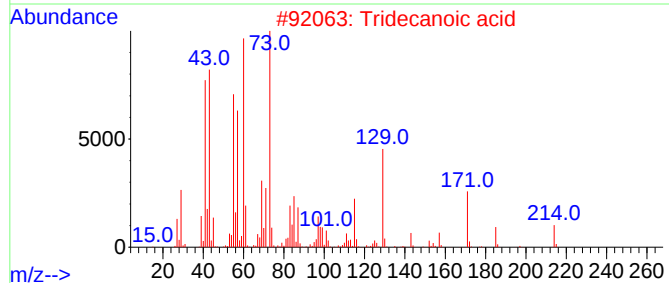
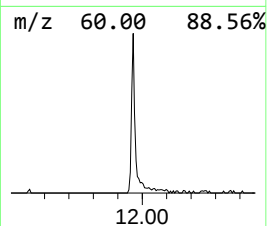
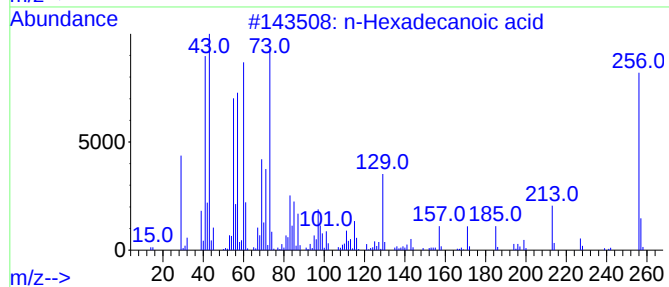
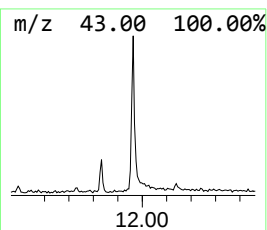
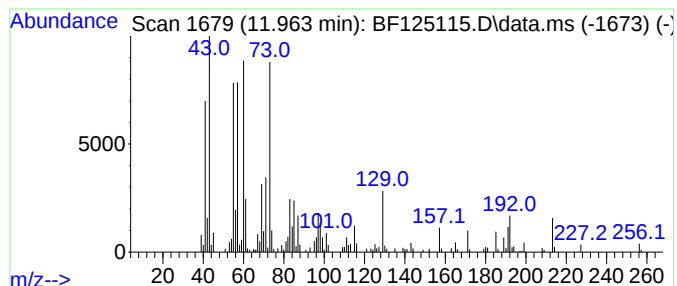
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	4.74 ng	411860	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125115.D
Acq On : 19 Aug 2021 15:33
Operator : JU/CG
Sample : M3449-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

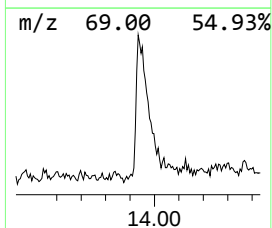
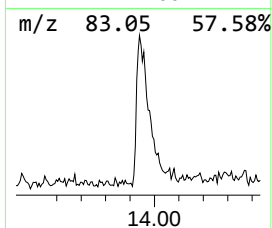
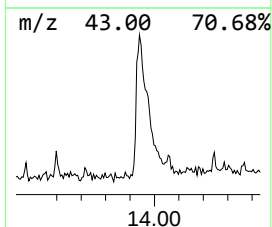
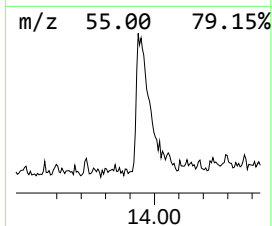
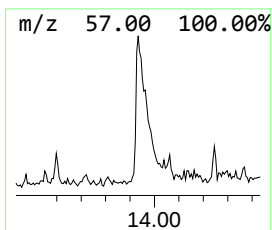
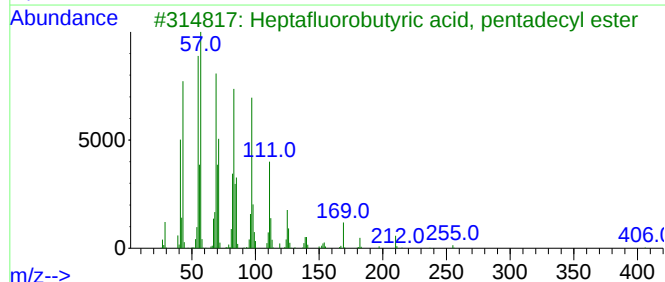
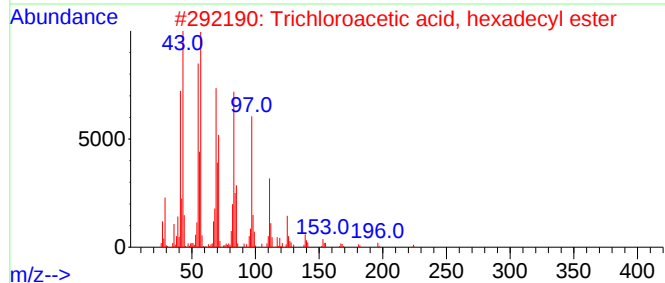
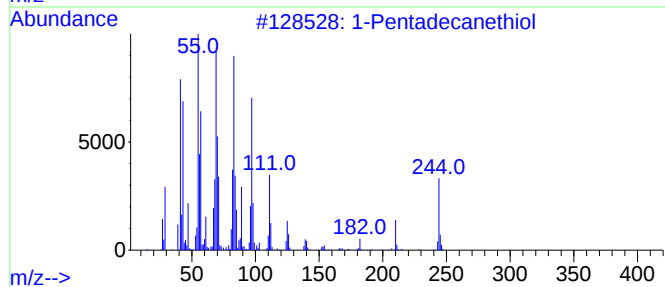
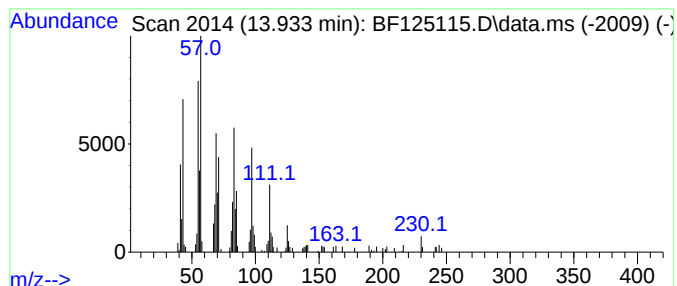
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Pentadecanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	6.81 ng	458289	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentadecanethiol	244	C15H32S	025276-70-4	95
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125115.D
Acq On : 19 Aug 2021 15:33
Operator : JU/CG
Sample : M3449-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

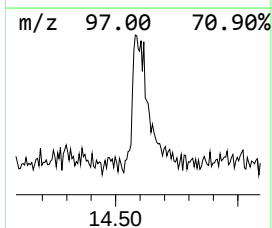
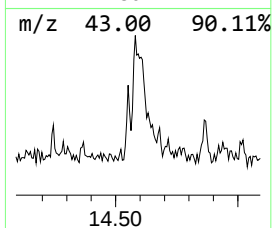
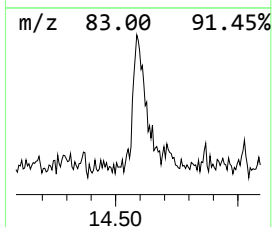
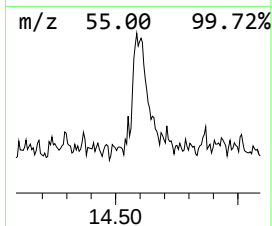
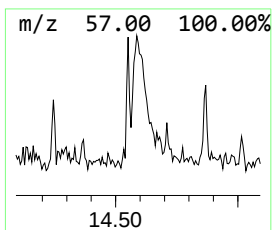
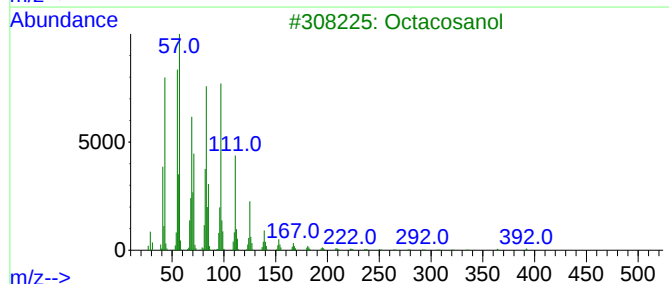
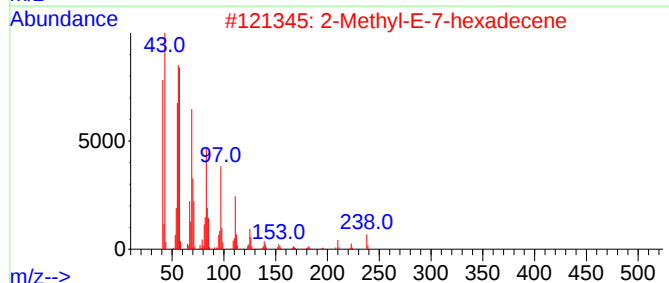
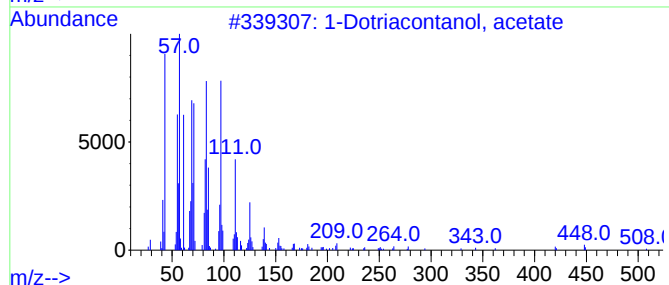
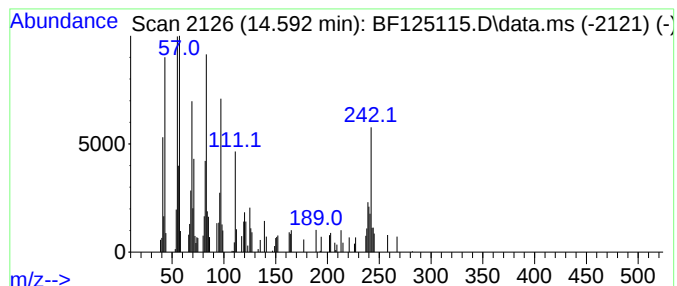
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Dotriacontanol, acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.592	2.39 ng	160611	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	58
2			2-Methyl-E-7-hexadecene	238	C17H34	064183-52-4	53
3			Octacosanol	410	C28H58O	000557-61-9	53
4			1-Heptadecene	238	C17H34	006765-39-5	52
5			Methyl 2-hydroxy-pentadecanoate	272	C16H32O3	1000336-35-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
Data File : BF125115.D
Acq On : 19 Aug 2021 15:33
Operator : JU/CG
Sample : M3449-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2

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...	2.234	35.9	ng	1999100	1	6.916	1112560	20.0
2-Pentanone, 4-...	5.151	3.1	ng	173197	1	6.916	1112560	20.0
Ethanol, 2-(2-b...	8.098	10.1	ng	748081	2	8.198	1483570	20.0
n-Hexadecanoic ...	11.963	4.7	ng	411860	4	11.445	1737960	20.0
1-Pentadecanethiol	13.933	6.8	ng	458289	5	14.080	1345690	20.0
1-Dotriacontano...	14.592	2.4	ng	160611	5	14.080	1345690	20.0