

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
 Data File : BF125522.D
 Acq On : 16 Sep 2021 00:53
 Operator : JU/CG
 Sample : M3687-25
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A015015

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-BF091521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125522.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	15	22	30	rVB	619265	784403	20.53%	3.101%
2	2.322	35	40	48	rBV2	33730	54657	1.43%	0.216%
3	4.469	384	405	408	rBV2	45740	214680	5.62%	0.849%
4	5.087	506	510	519	rBV	439625	492228	12.88%	1.946%
5	5.492	575	579	595	rBV	1938864	1791396	46.89%	7.081%
6	6.498	746	750	769	rBV	2263470	2484663	65.03%	9.822%
7	6.863	809	812	816	rBV	1208468	1036230	27.12%	4.096%
8	7.428	903	908	911	rBV	1672795	1598503	41.84%	6.319%
9	7.545	924	928	937	rBV3	40158	91830	2.40%	0.363%
10	7.898	985	988	995	rBV	41574	94446	2.47%	0.373%
11	8.057	1011	1015	1026	rBV2	130121	285264	7.47%	1.128%
12	8.151	1026	1031	1034	rBV	1447302	1349891	35.33%	5.336%
13	8.504	1088	1091	1113	rBV	102942	199353	5.22%	0.788%
14	9.074	1185	1188	1197	rBV2	43108	94493	2.47%	0.374%
15	9.227	1208	1214	1217	rBV	3906994	3721906	97.42%	14.712%
16	9.333	1228	1232	1236	rVB2	43776	57865	1.51%	0.229%
17	9.904	1324	1329	1333	rBV	1599098	1497984	39.21%	5.921%
18	10.698	1460	1464	1473	rBV	1379919	1331943	34.86%	5.265%
19	10.804	1478	1482	1486	rVB	75635	90445	2.37%	0.358%
20	11.251	1554	1558	1560	rBV	91715	80311	2.10%	0.317%
21	11.398	1579	1583	1586	rBV	1524598	1418590	37.13%	5.608%
22	11.674	1628	1630	1633	rBV	86468	71056	1.86%	0.281%
23	11.780	1645	1648	1652	rVB	83870	69357	1.82%	0.274%
24	11.921	1669	1672	1676	rBV5	26509	49932	1.31%	0.197%
25	12.086	1697	1700	1702	rVB	70845	53821	1.41%	0.213%
26	12.486	1763	1768	1770	rBV2	140309	168391	4.41%	0.666%
27	12.574	1780	1783	1786	rBV2	40439	40478	1.06%	0.160%
28	12.845	1826	1829	1831	rBV2	56882	43918	1.15%	0.174%
29	12.986	1848	1853	1856	rBV	4036421	3820589	100.00%	15.102%
30	13.204	1887	1890	1893	rVB2	64677	56861	1.49%	0.225%
31	13.545	1945	1948	1951	rBV3	69211	71127	1.86%	0.281%
32	13.874	2001	2004	2006	rBV2	71070	60476	1.58%	0.239%
33	13.904	2006	2009	2011	rBV	64052	53498	1.40%	0.211%
34	14.039	2028	2032	2036	rBV	1035586	869759	22.77%	3.438%
35	14.192	2055	2058	2062	rVB	62377	55140	1.44%	0.218%
36	14.498	2107	2110	2112	rVB	56754	49078	1.28%	0.194%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125522.D
Acq On : 16 Sep 2021 00:53
Operator : JU/CG
Sample : M3687-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A015015

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-BF091521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.804	2160	2162	2165	rVB2	42259	40412	1.06%	0.160%
38	15.145	2218	2220	2224	rVB	50832	50213	1.31%	0.198%
39	15.527	2279	2285	2293	rVB	663666	902796	23.63%	3.569%

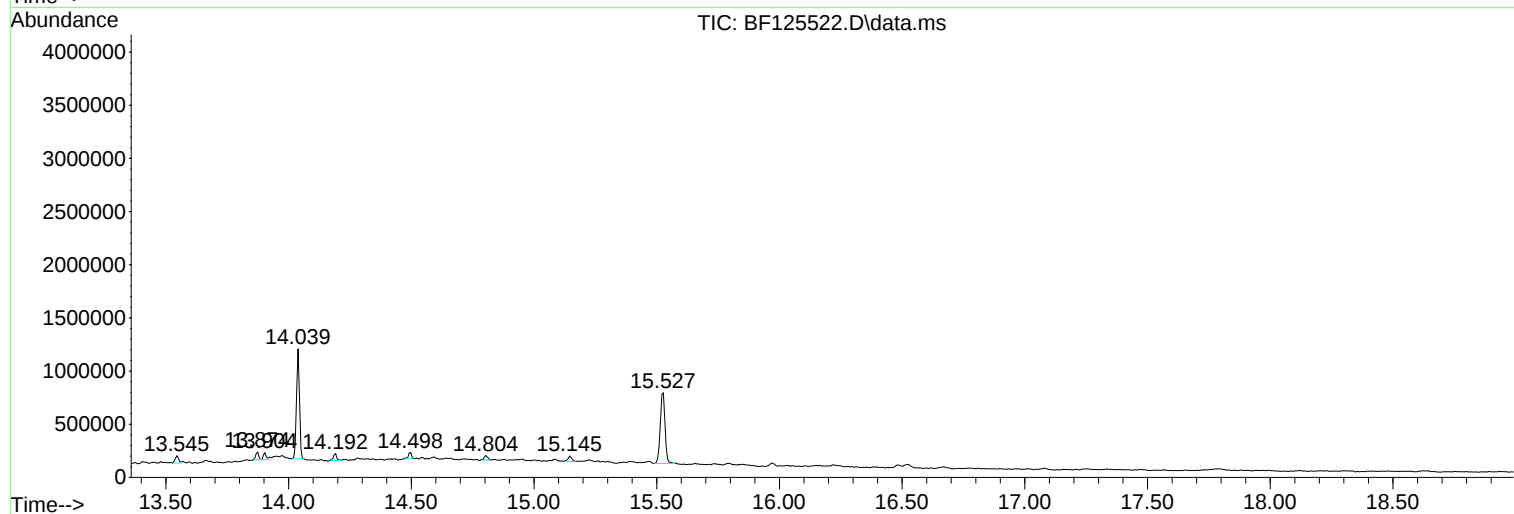
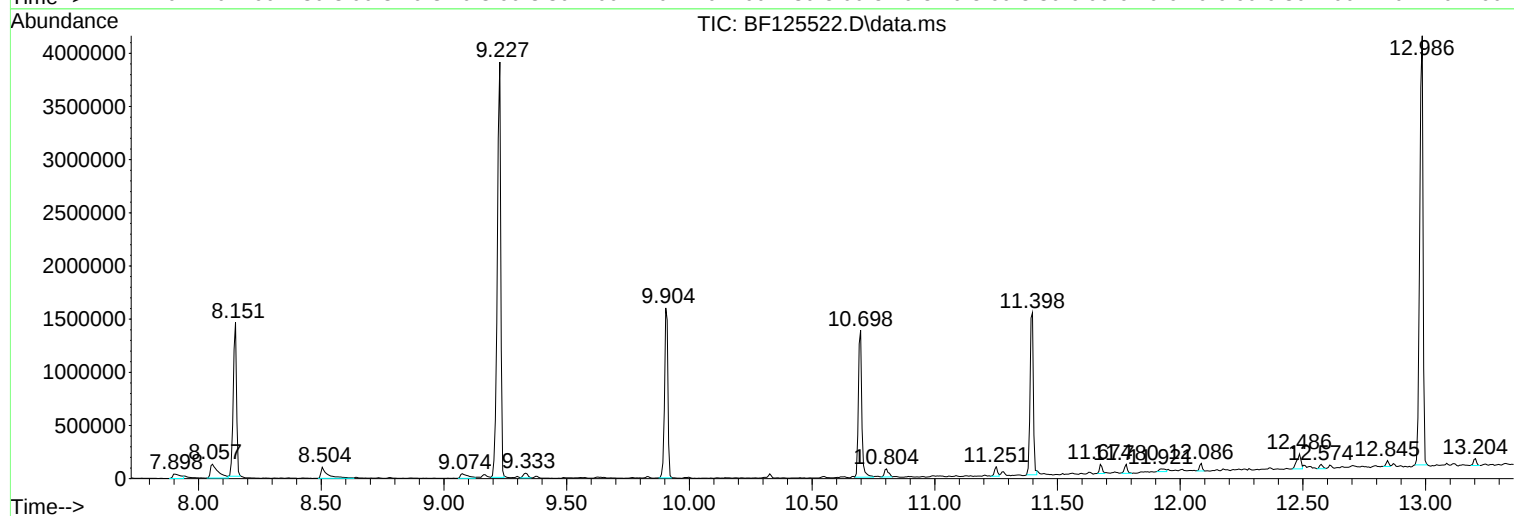
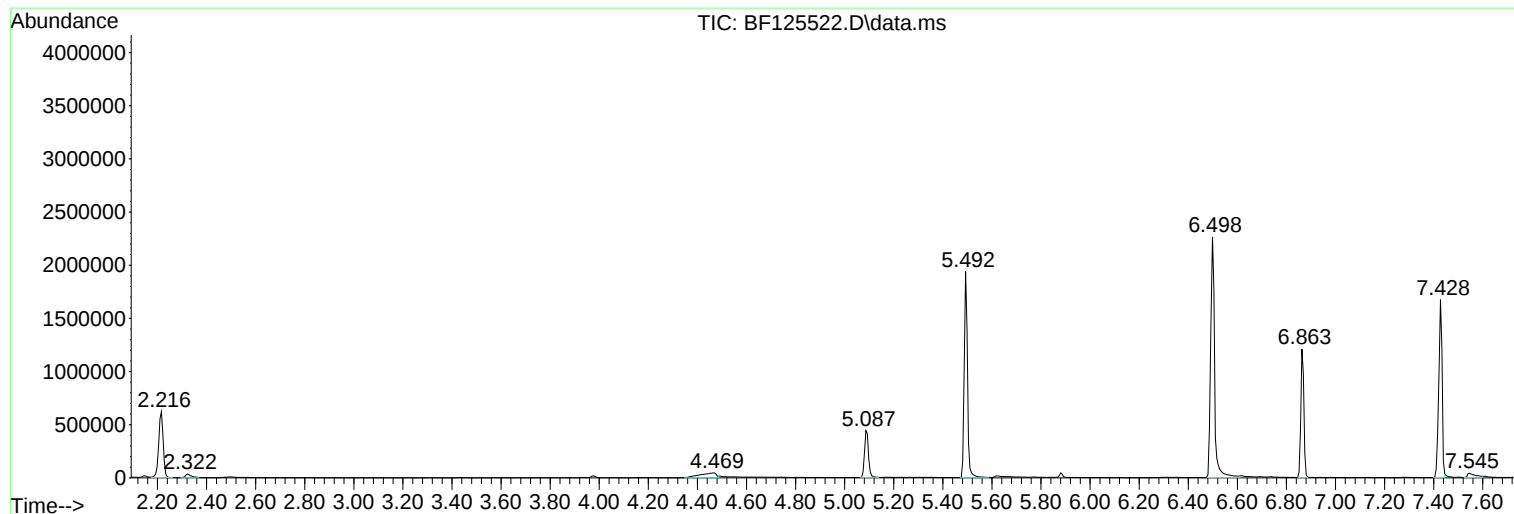
Sum of corrected areas: 25297983

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125522.D
Acq On : 16 Sep 2021 00:53
Operator : JU/CG
Sample : M3687-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A015015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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\BF091521\
Data File : BF125522.D
Acq On : 16 Sep 2021 00:53
Operator : JU/CG
Sample : M3687-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A015015

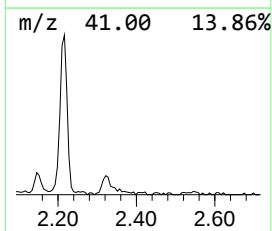
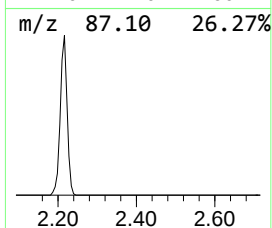
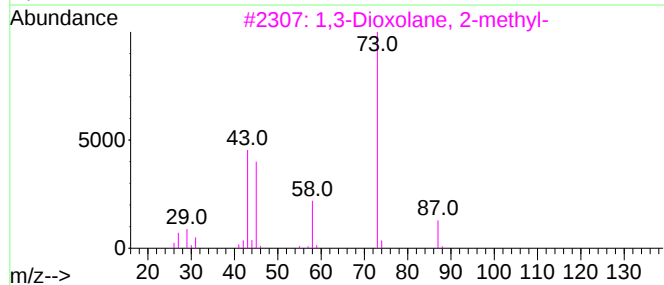
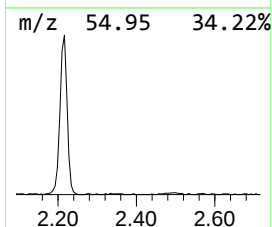
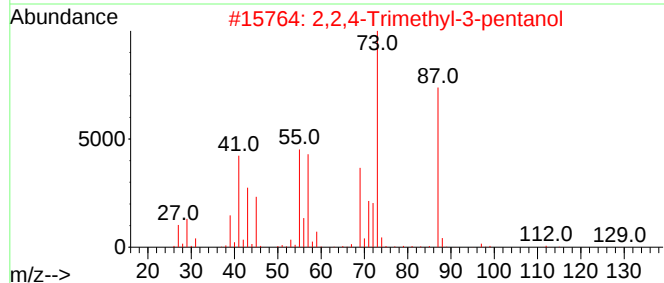
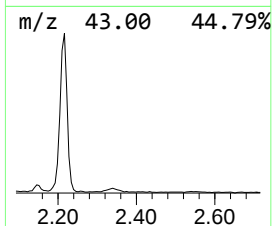
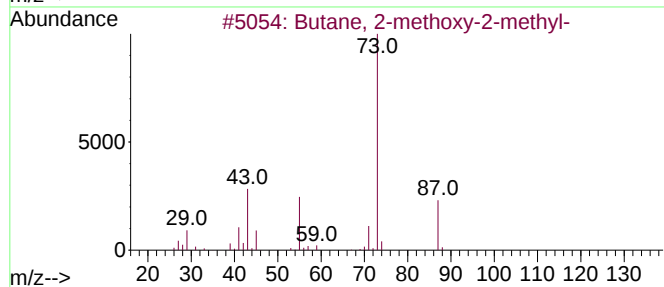
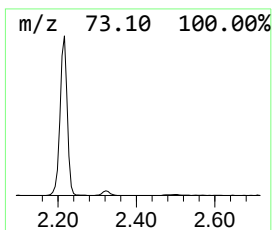
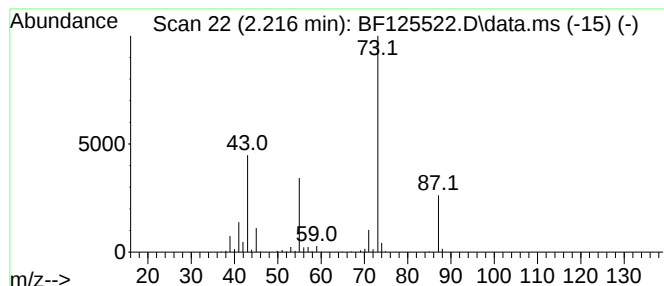
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.216	15.14 ng	784403	1,4-Dichlorobenzene-d4	6.863

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125522.D
Acq On : 16 Sep 2021 00:53
Operator : JU/CG
Sample : M3687-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A015015

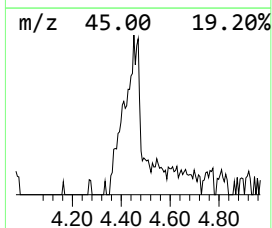
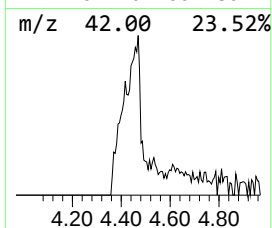
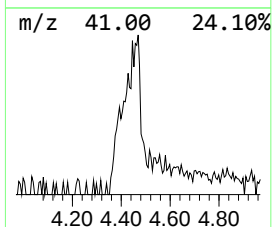
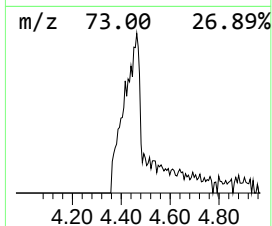
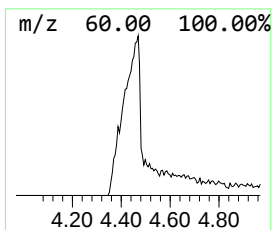
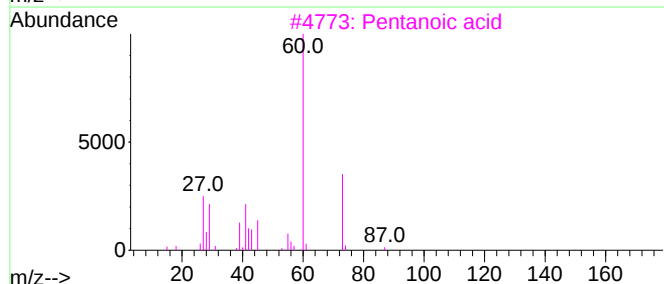
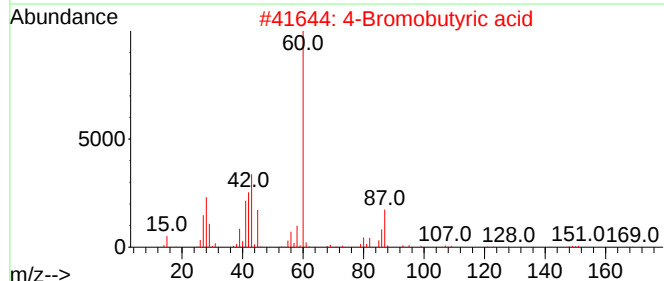
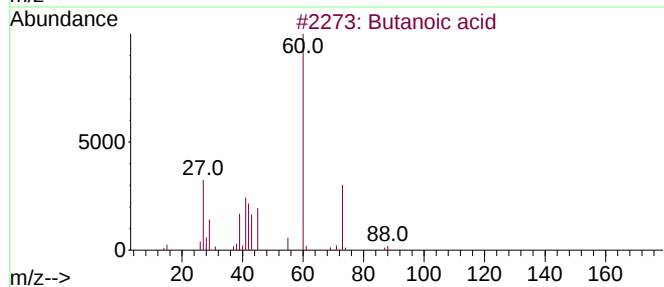
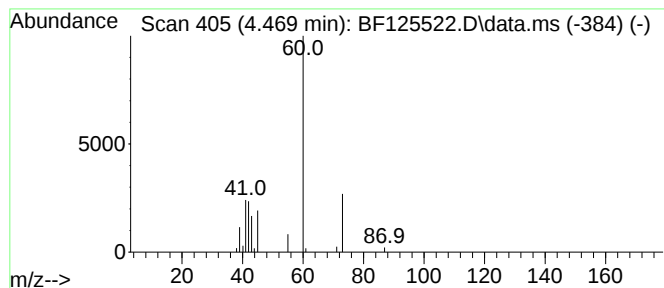
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.469	4.14 ng	214680	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	83
2			4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9
3			Pentanoic acid	102	C5H10O2	000109-52-4	9
4			Isobutylamine	73	C4H11N	000078-81-9	7
5			Formamidoxime	60	CH4N2O	000624-82-8	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125522.D
Acq On : 16 Sep 2021 00:53
Operator : JU/CG
Sample : M3687-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

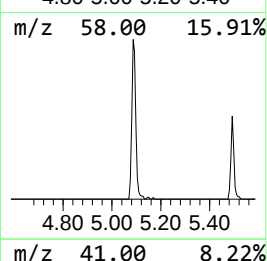
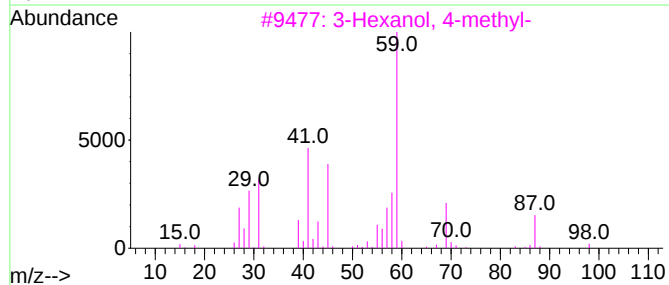
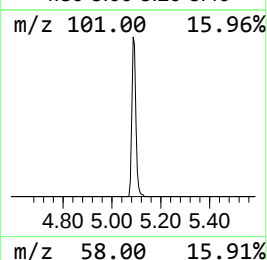
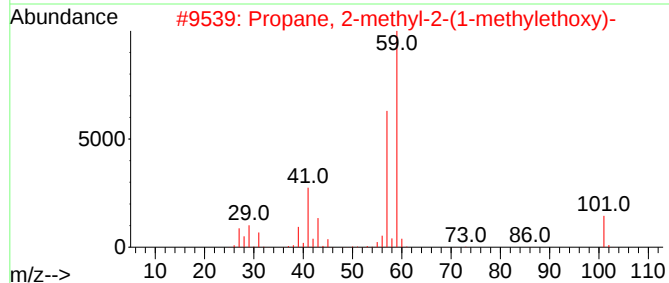
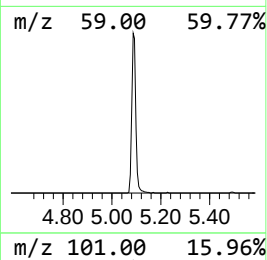
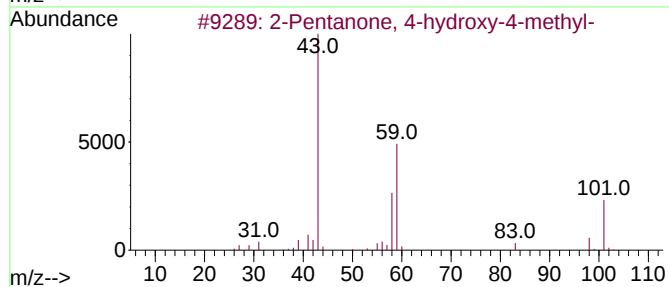
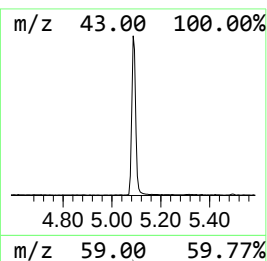
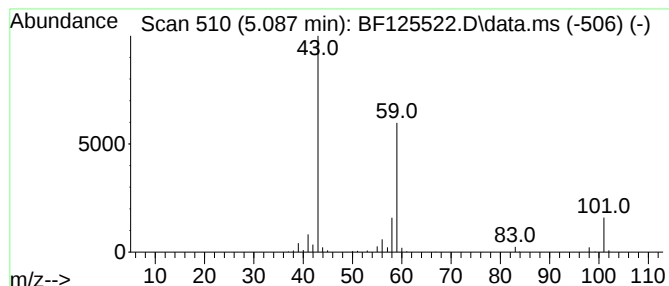
Instrument :
BNA_F
ClientSampleId :
A015015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.087	9.50 ng	492228	1,4-Dichlorobenzene-d4			6.863
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
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	33
5	3-Octanol		130	C8H18O	000589-98-0	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125522.D
Acq On : 16 Sep 2021 00:53
Operator : JU/CG
Sample : M3687-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A015015

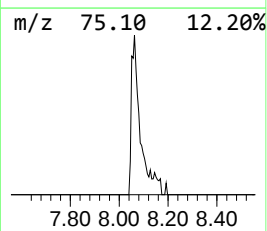
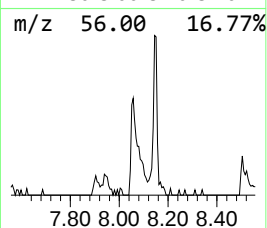
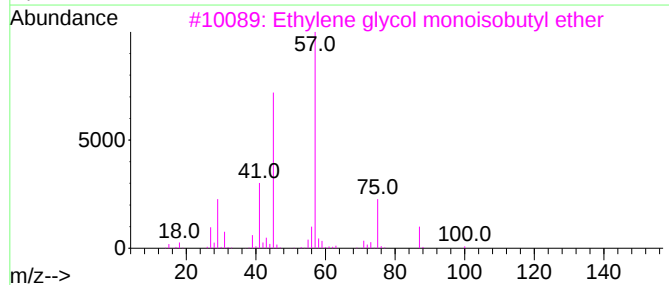
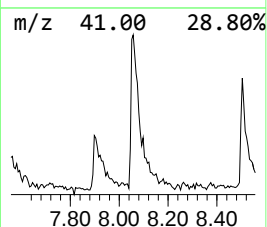
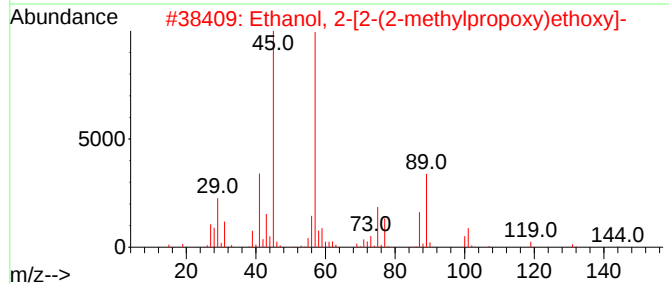
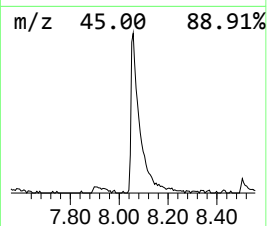
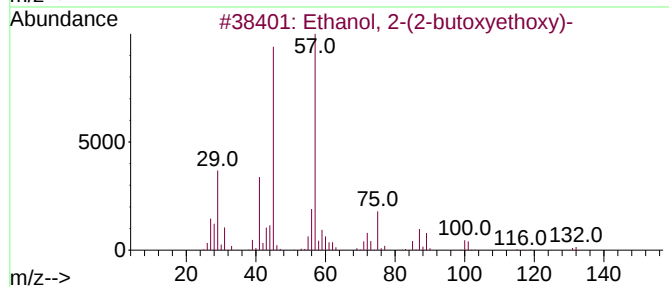
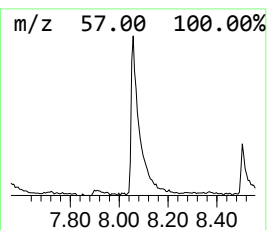
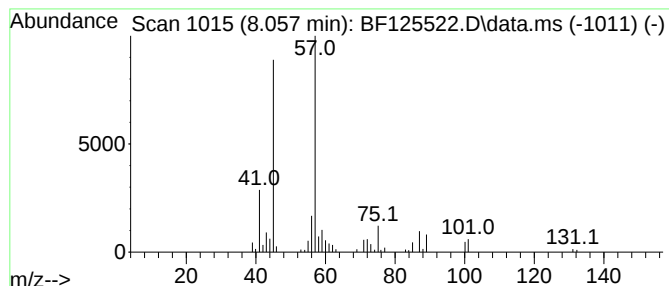
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.057	4.23 ng	285264	Naphthalene-d8	8.151

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	72
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125522.D
Acq On : 16 Sep 2021 00:53
Operator : JU/CG
Sample : M3687-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A015015

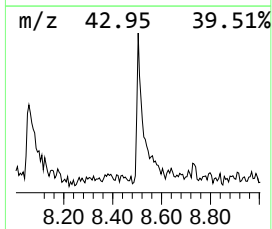
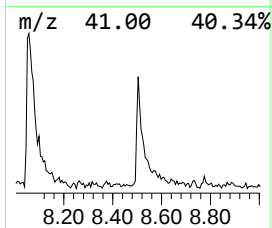
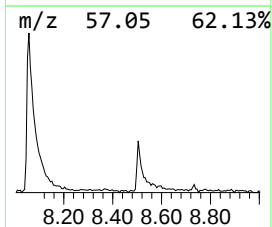
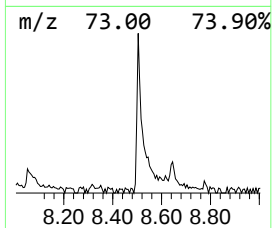
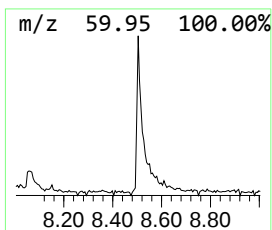
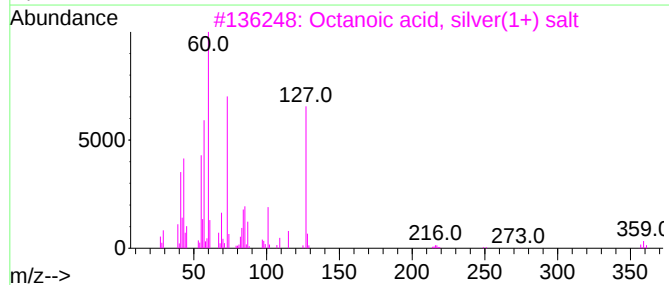
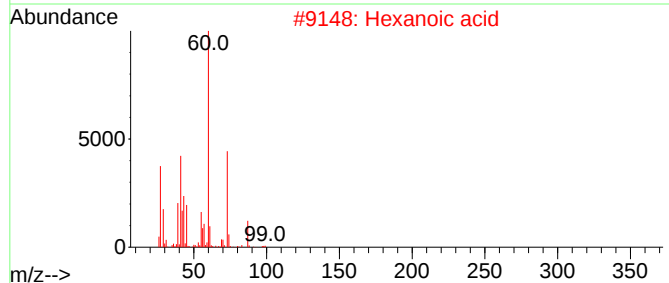
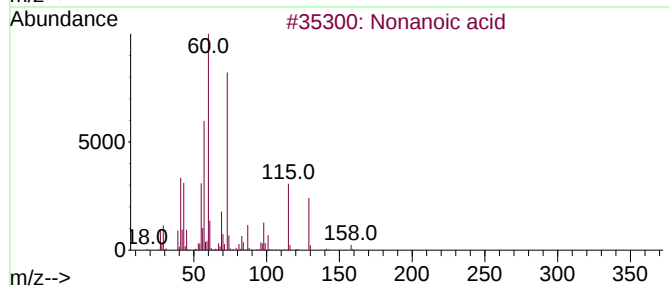
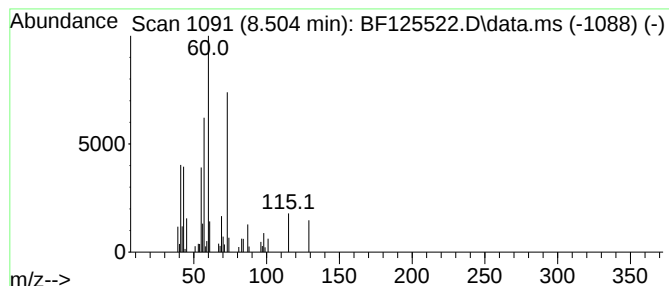
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Nonanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.504	2.95 ng	199353	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	83
2			Hexanoic acid	116	C6H12O2	000142-62-1	59
3			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	59
4			Octanoic acid	144	C8H16O2	000124-07-2	59
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125522.D
Acq On : 16 Sep 2021 00:53
Operator : JU/CG
Sample : M3687-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A015015

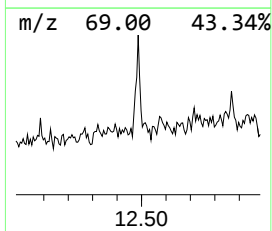
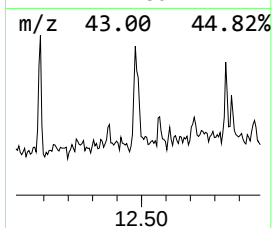
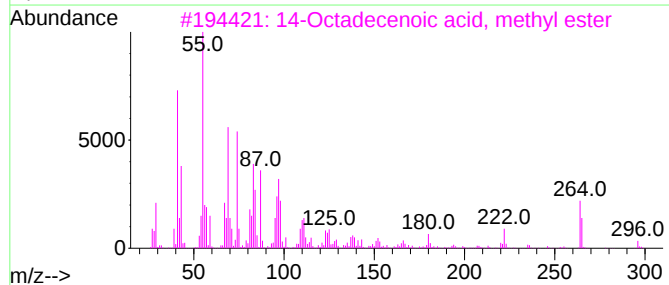
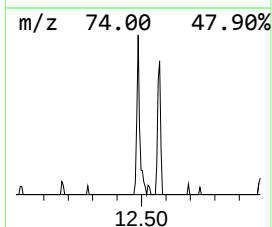
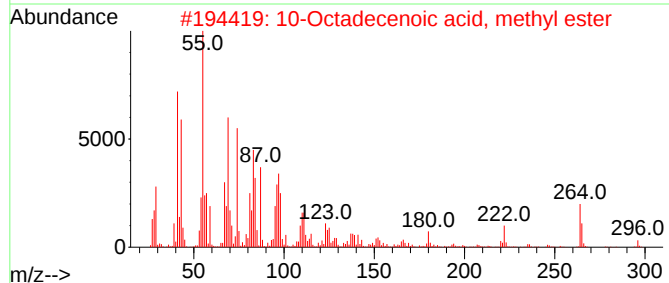
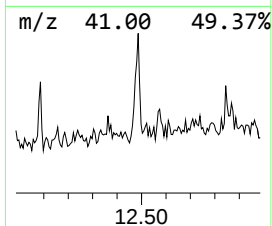
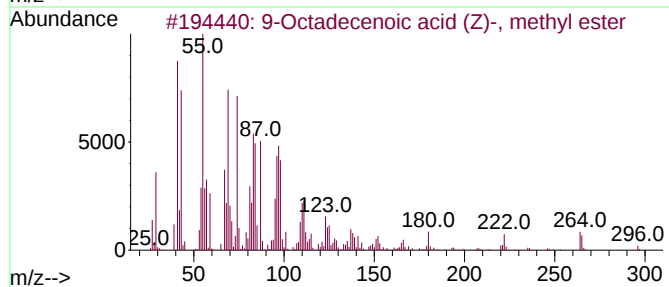
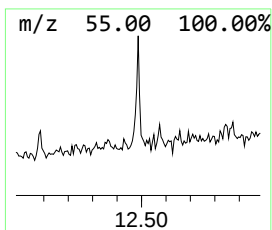
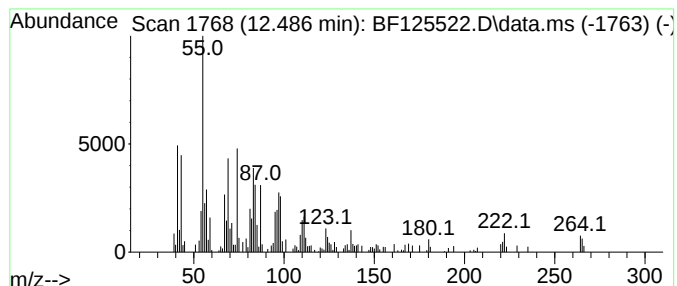
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.486	2.37 ng	168391	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
3			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
4			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90
5			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125522.D
Acq On : 16 Sep 2021 00:53
Operator : JU/CG
Sample : M3687-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A015015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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...	2.216	15.1	ng	784403	1	6.863	1036230	20.0
Butanoic acid	4.469	4.1	ng	214680	1	6.863	1036230	20.0
2-Pentanone, 4-...	5.087	9.5	ng	492228	1	6.863	1036230	20.0
Ethanol, 2-(2-b...	8.057	4.2	ng	285264	2	8.151	1349890	20.0
Nonanoic acid	8.504	3.0	ng	199353	2	8.151	1349890	20.0
9-Octadecenoic ...	12.486	2.4	ng	168391	4	11.398	1418590	20.0