

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
 Data File : BF125546.D
 Acq On : 21 Sep 2021 20:44
 Operator : JU/CG
 Sample : M3835-03
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-CB-04-(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: BF125546.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	13	rVB	84971	93392	1.28%	0.144%
2	2.204	13	20	28	rVB	3261775	4250901	58.39%	6.554%
3	3.393	219	222	239	rBV	55177	135473	1.86%	0.209%
4	4.004	322	326	332	rVB	375286	456402	6.27%	0.704%
5	5.110	496	514	517	rBV2	92562	232502	3.19%	0.358%
6	5.210	527	531	535	rBV	326962	338029	4.64%	0.521%
7	5.292	543	545	547	rVB	189156	129152	1.77%	0.199%
8	5.510	577	582	585	rBV	2413211	2214847	30.42%	3.415%
9	6.175	679	695	697	rBV	71259	212131	2.91%	0.327%
10	6.504	747	751	756	rBV	1567354	1476941	20.29%	2.277%
11	6.892	814	817	822	rBV	1315561	1234273	16.95%	1.903%
12	6.945	822	826	829	rVB2	69012	102764	1.41%	0.158%
13	7.057	842	845	851	rVB3	83194	108891	1.50%	0.168%
14	7.286	879	884	889	rBV	1526270	1329233	18.26%	2.049%
15	7.457	907	913	916	rBV	3257856	3140007	43.13%	4.841%
16	7.575	929	933	934	rBV2	82240	98094	1.35%	0.151%
17	7.598	934	937	938	rVV2	157920	201190	2.76%	0.310%
18	7.628	938	942	944	rVV2	276131	479319	6.58%	0.739%
19	7.722	944	958	960	rVB2	866890	2650345	36.40%	4.086%
20	7.945	983	996	999	rBV	5880661	7280546	100.00%	11.225%
21	8.081	1016	1019	1023	rBV	1021455	781704	10.74%	1.205%
22	8.175	1031	1035	1037	rBV	1693598	1660794	22.81%	2.561%
23	8.198	1037	1039	1043	rVB	1574113	1227366	16.86%	1.892%
24	8.428	1069	1078	1081	rBV	516850	849215	11.66%	1.309%
25	8.522	1090	1094	1098	rBV4	62537	81082	1.11%	0.125%
26	8.698	1121	1124	1129	rBV2	188917	210612	2.89%	0.325%
27	8.910	1155	1160	1162	rBV	378035	415026	5.70%	0.640%
28	9.016	1162	1178	1180	rVB	1893447	5447795	74.83%	8.399%
29	9.257	1214	1219	1222	rVB	6487384	6059537	83.23%	9.342%
30	9.357	1231	1236	1240	rBV2	142317	150348	2.07%	0.232%
31	9.469	1253	1255	1260	rVB3	57434	84054	1.15%	0.130%
32	9.822	1311	1315	1319	rBV	244106	238022	3.27%	0.367%
33	9.904	1325	1329	1331	rBV	190619	180777	2.48%	0.279%
34	9.933	1331	1334	1337	rVB	2268348	1829219	25.12%	2.820%
35	10.222	1379	1383	1386	rVB2	80586	94552	1.30%	0.146%
36	10.392	1409	1412	1414	rBV	88172	74933	1.03%	0.116%

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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

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37	10.563	1437	1441	1443	rBV	343316	276276	3.79%	0.426%
38	10.663	1455	1458	1462	rBV2	95352	101733	1.40%	0.157%
39	10.722	1462	1468	1471	rBV	3888696	3613784	49.64%	5.572%
40	10.822	1478	1485	1489	rBV	876669	1071364	14.72%	1.652%
41	10.863	1489	1492	1496	rVB	308069	282800	3.88%	0.436%
42	10.904	1496	1499	1502	rBV	572802	438901	6.03%	0.677%
43	11.133	1533	1538	1549	rBV	705531	921342	12.65%	1.421%
44	11.416	1582	1586	1590	rBV	1995421	1766451	24.26%	2.723%
45	11.498	1597	1600	1604	rBV	151497	128545	1.77%	0.198%
46	11.945	1672	1676	1685	rBV2	787124	703933	9.67%	1.085%
47	12.727	1806	1809	1817	rBV	571771	623288	8.56%	0.961%
48	12.868	1830	1833	1838	rBV	296335	294812	4.05%	0.455%
49	13.004	1852	1856	1860	rBV	5148781	5145180	70.67%	7.933%
50	13.474	1933	1936	1941	rVB	95561	98388	1.35%	0.152%
51	13.833	1994	1997	1999	rBV3	82051	84124	1.16%	0.130%
52	13.898	2004	2008	2011	rBV2	537362	536133	7.36%	0.827%
53	14.051	2030	2034	2038	rBV	1272226	1175357	16.14%	1.812%
54	14.533	2113	2116	2121	rBV	86843	75195	1.03%	0.116%
55	14.745	2149	2152	2160	rVB2	74656	82879	1.14%	0.128%
56	15.451	2268	2272	2281	rVV3	136285	190460	2.62%	0.294%
57	15.533	2281	2286	2290	rVV	945007	1135770	15.60%	1.751%
58	16.074	2374	2378	2385	rVB2	50360	77605	1.07%	0.120%
59	16.374	2423	2429	2435	rBV3	108258	179185	2.46%	0.276%
60	17.221	2569	2573	2583	rVB9	51983	118999	1.63%	0.183%
61	17.633	2637	2643	2650	rVB5	86696	188020	2.58%	0.290%

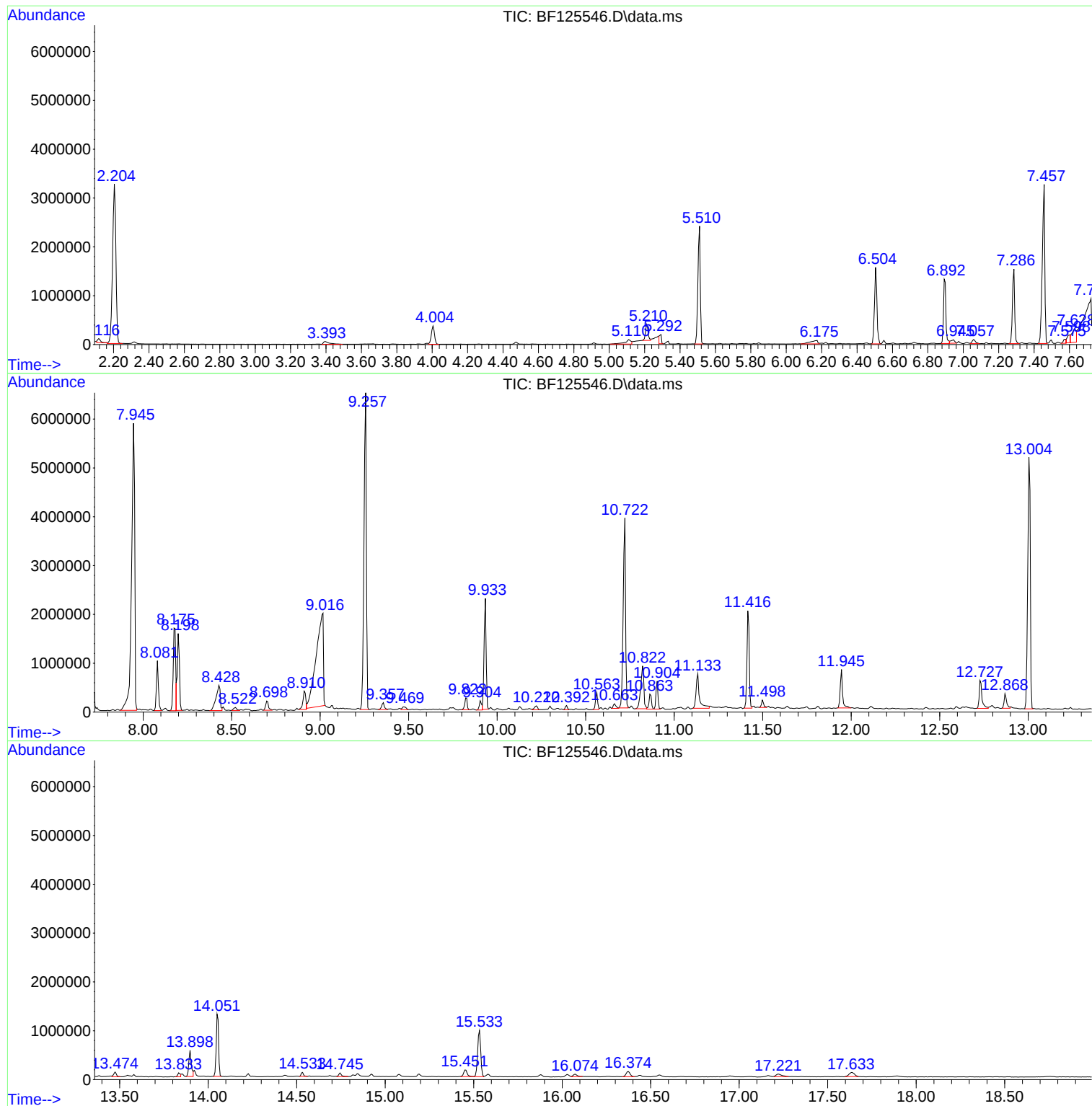
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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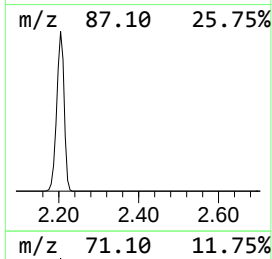
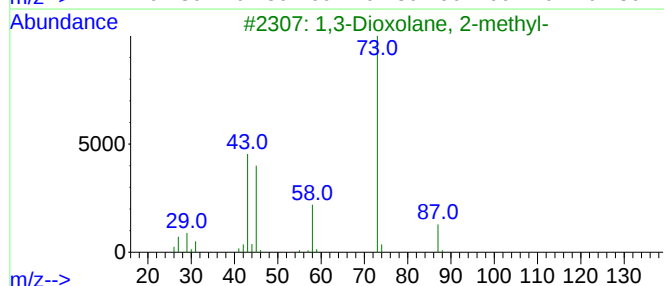
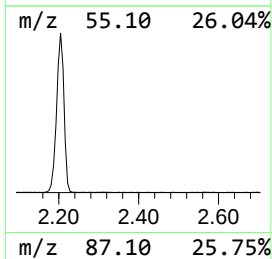
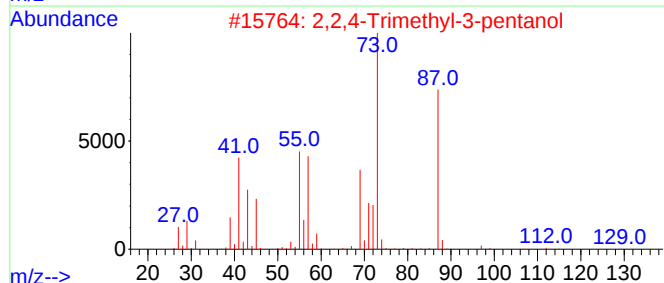
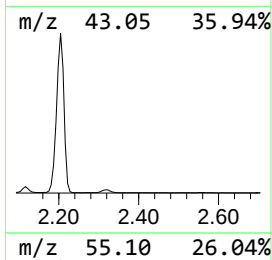
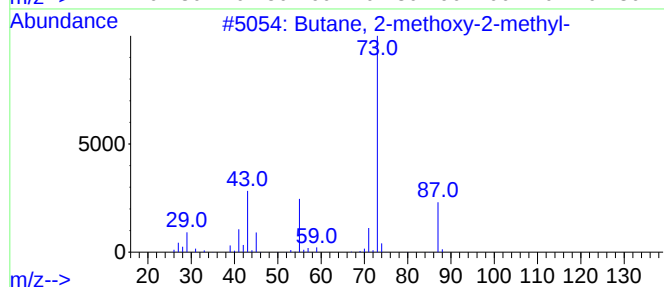
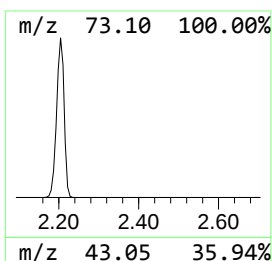
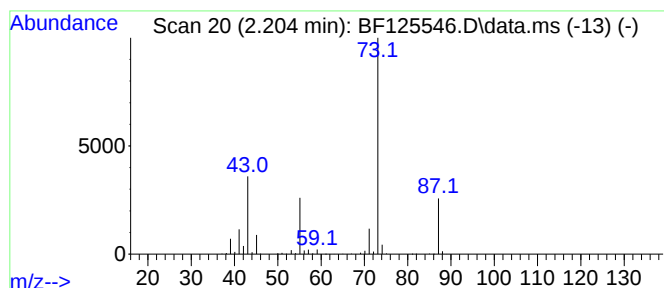
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	68.88 ng	4250900	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



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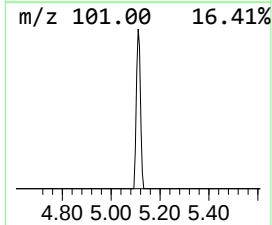
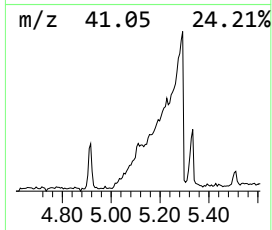
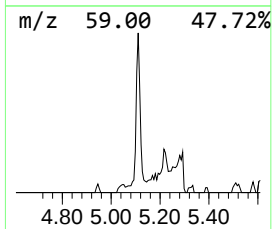
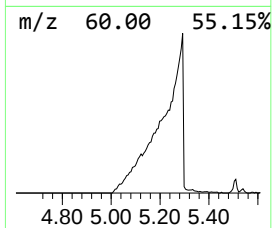
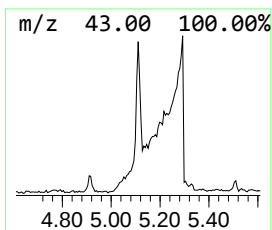
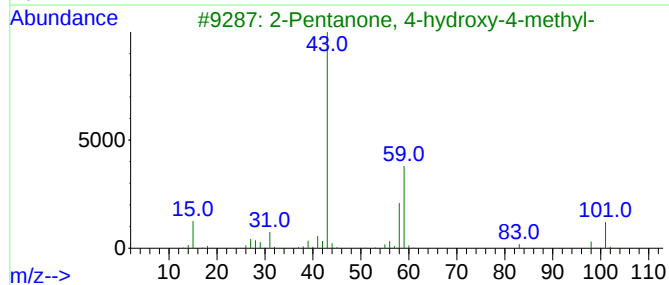
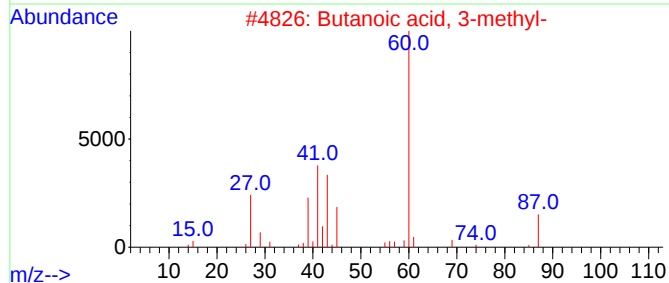
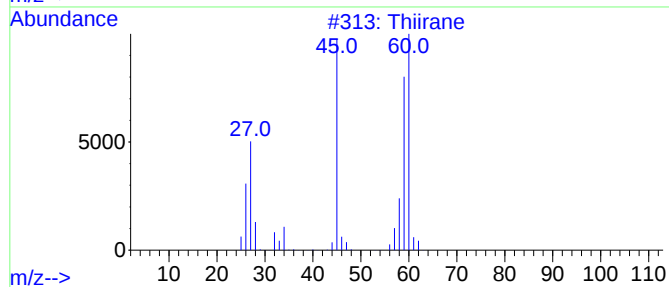
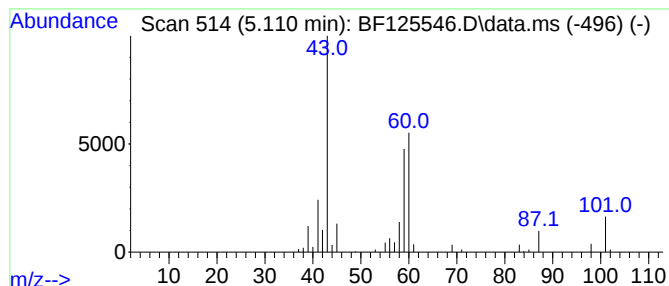
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown5.110 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	3.77 ng	232502	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiirane	60	C2H4S	000420-12-2	47
2			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	38
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
4			Hexanoic acid	116	C6H12O2	000142-62-1	25
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23



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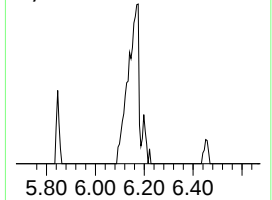
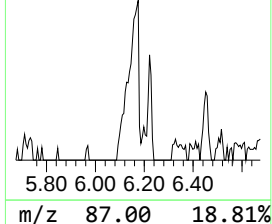
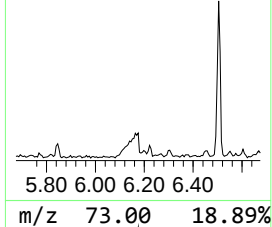
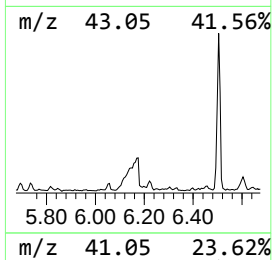
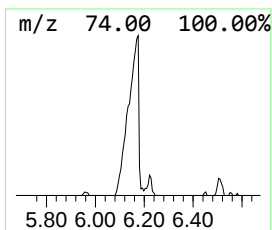
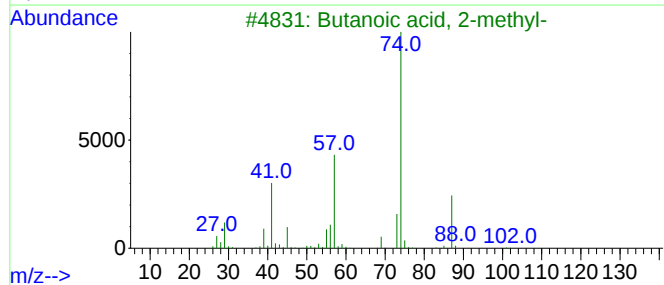
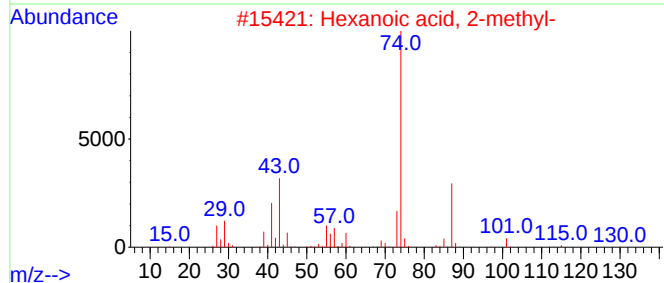
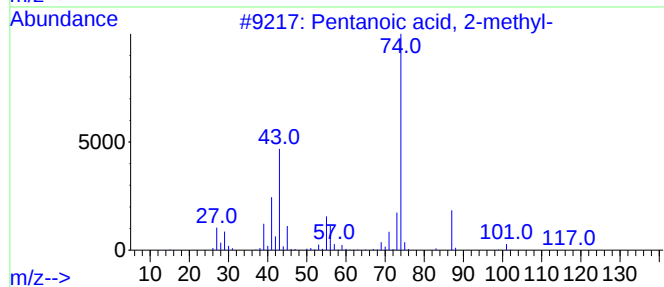
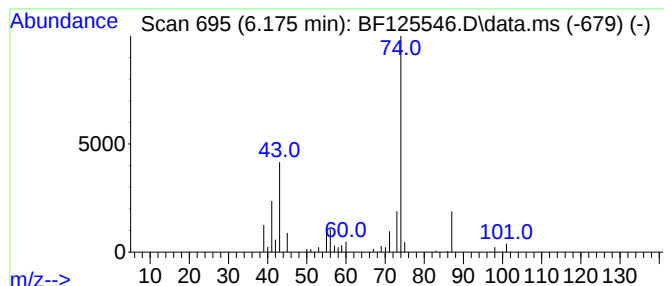
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentanoic acid, 2-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.175	3.44 ng	212131	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	83
2			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	50
3			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	45
4			2,3-Dimethylpentanoic acid	130	C7H14O2	082608-03-5	38
5			2-Methylheptanoic acid	144	C8H16O2	001188-02-9	38



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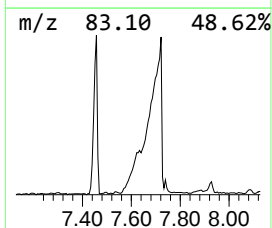
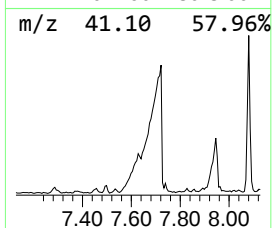
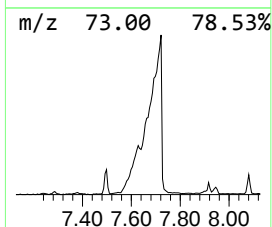
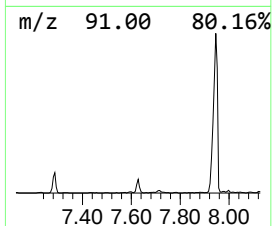
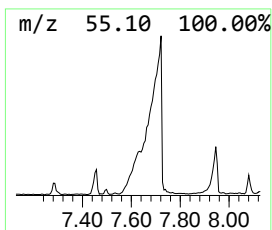
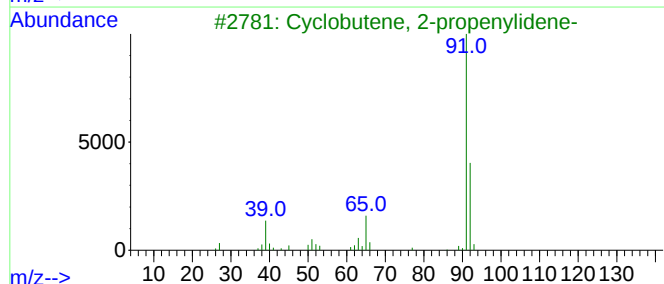
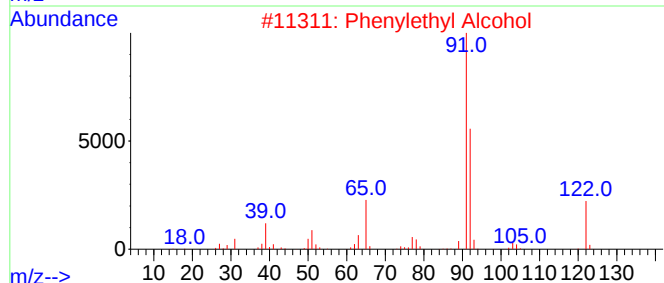
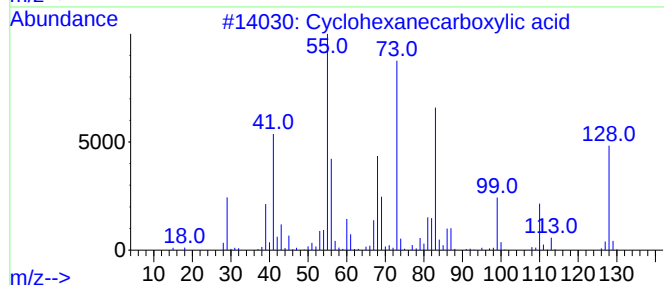
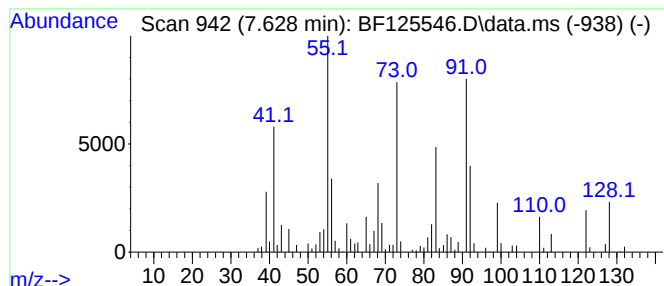
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexanecarboxylic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.628	5.77 ng	479319	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	90
2			Phenylethyl Alcohol	122	C8H10O	000060-12-8	30
3			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	11
4			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	11
5			Toluene	92	C7H8	000108-88-3	10



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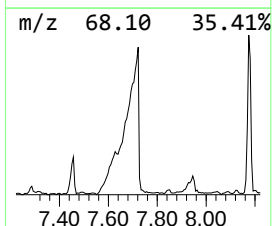
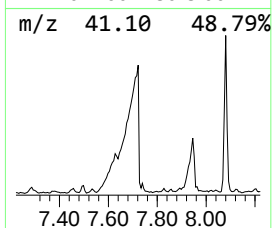
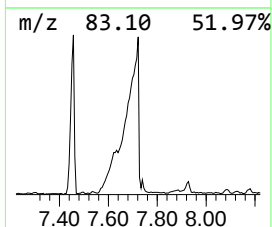
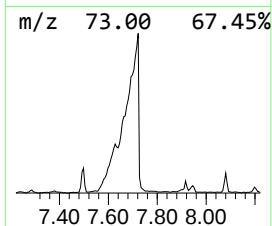
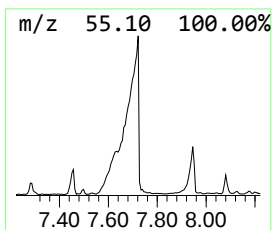
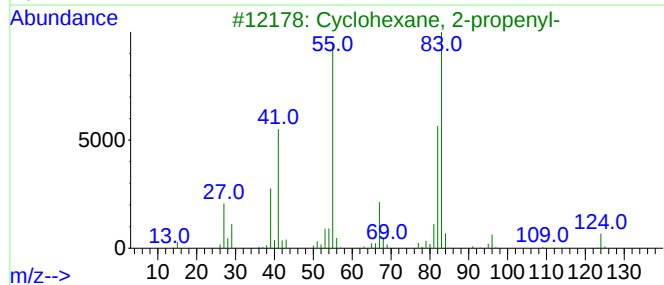
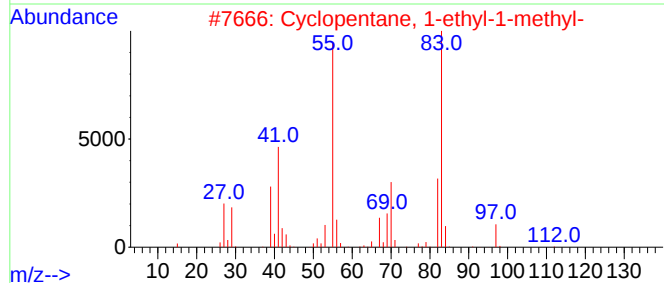
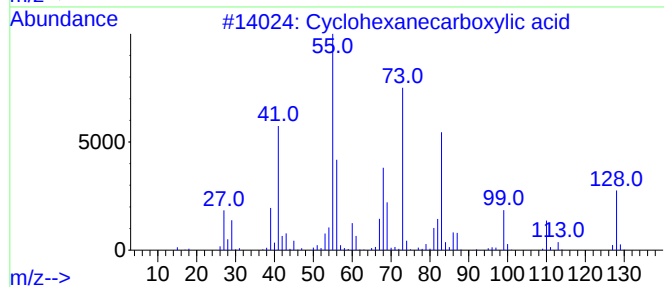
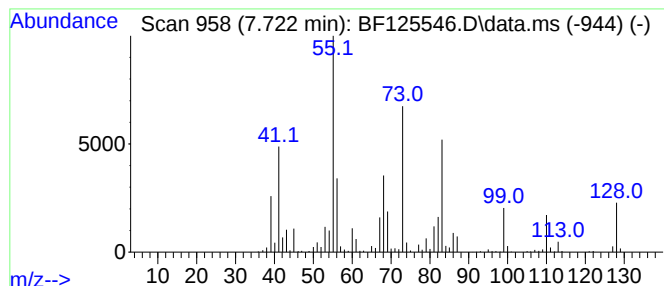
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown7.722 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.722	31.92 ng	2650350	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	97
2			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	27
3			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	27
4			Trichloroacetic acid, 6-chlorohe...	280	C8H12Cl4O2	1000330-89-2	27
5			3,4-Dihydro-2H-pyran-2-carboxyli...	128	C6H8O3	1010132-10-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
Operator : JU/CG
Sample : M3835-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-04-(1.0)

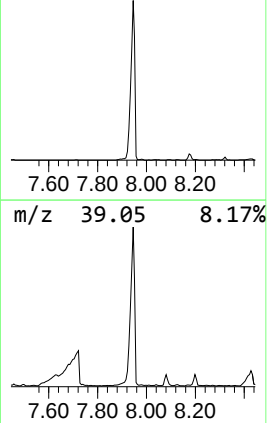
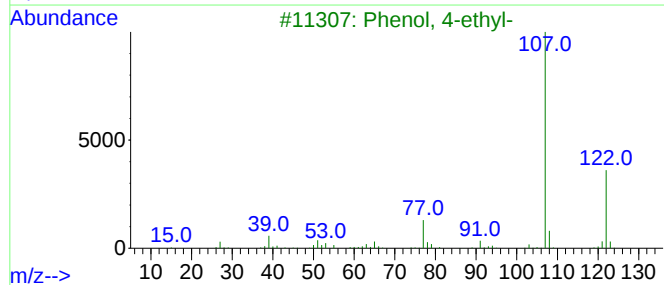
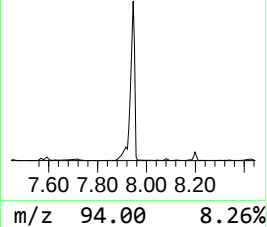
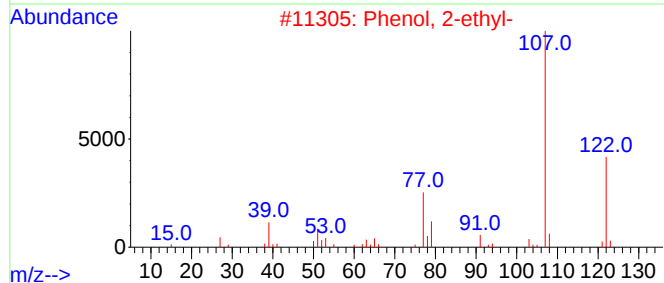
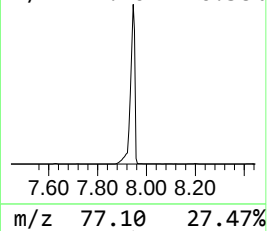
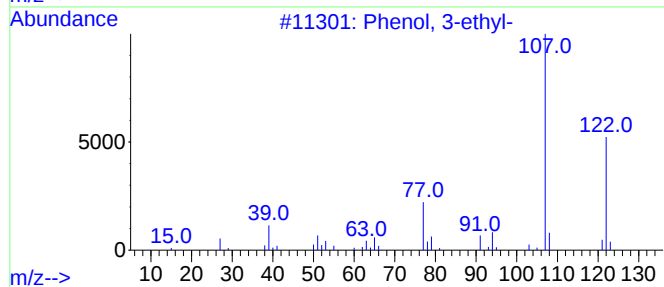
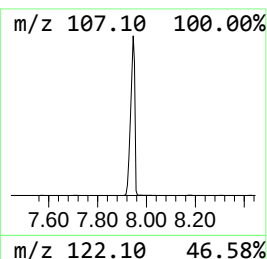
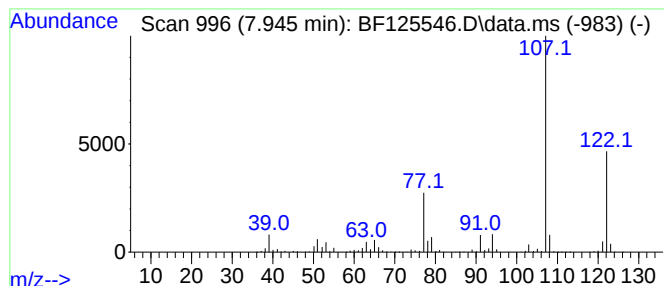
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 3-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.945	87.68 ng	7280550	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 3-ethyl-	122	C8H10O	000620-17-7	97
2			Phenol, 2-ethyl-	122	C8H10O	000090-00-6	91
3			Phenol, 4-ethyl-	122	C8H10O	000123-07-9	91
4			Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8	78
5			5-Acetylpyrimidine	122	C6H6N2O	010325-70-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
Operator : JU/CG
Sample : M3835-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-04-(1.0)

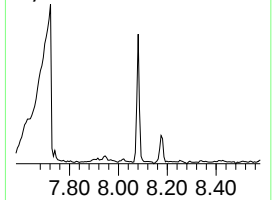
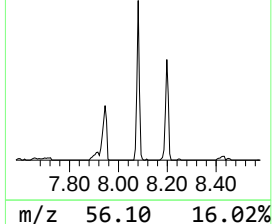
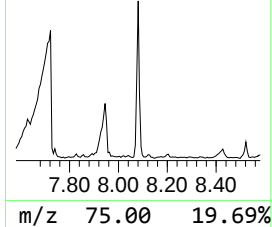
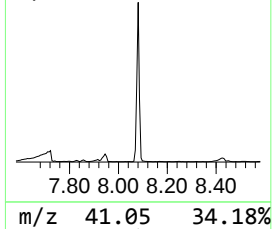
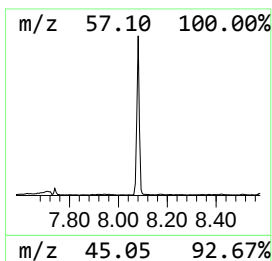
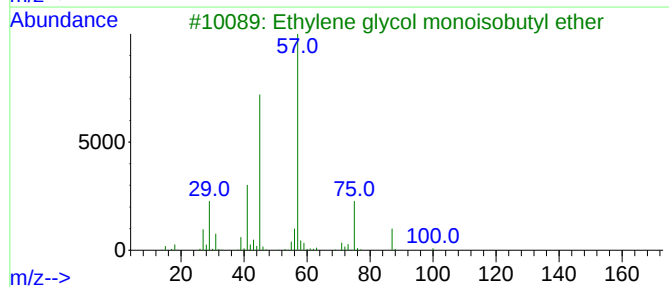
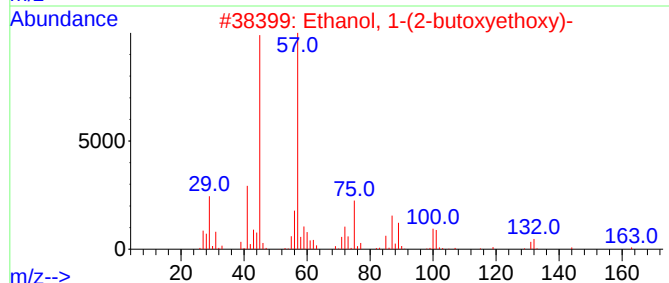
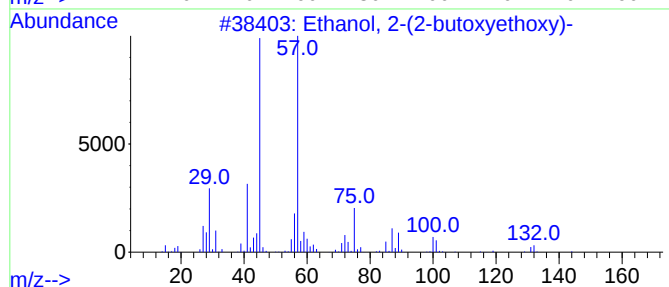
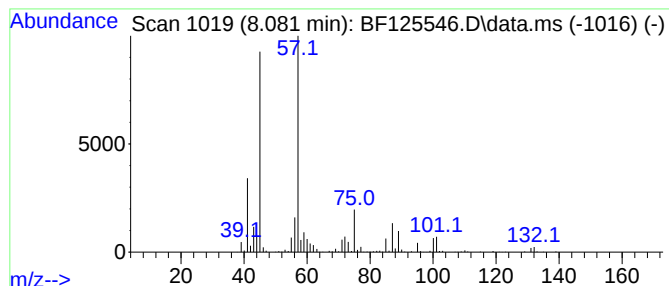
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.081	9.41 ng	781704	Naphthalene-d8	8.181

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			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	53
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
Operator : JU/CG
Sample : M3835-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-CB-04-(1.0)

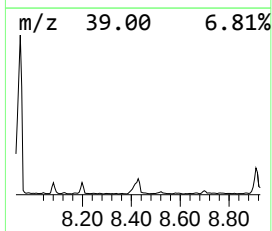
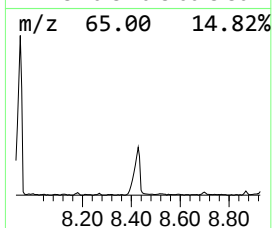
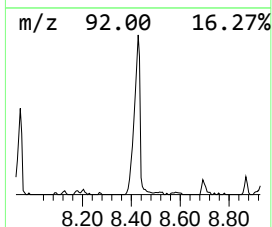
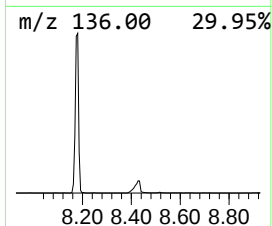
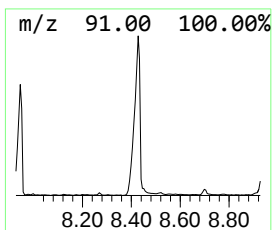
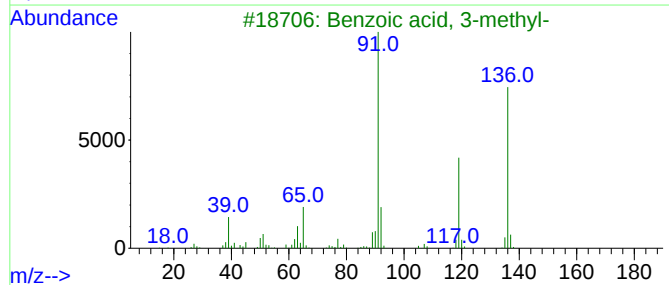
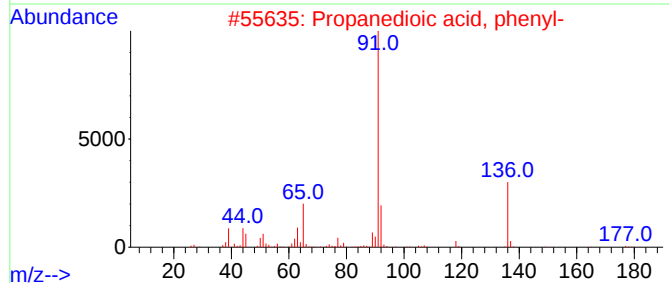
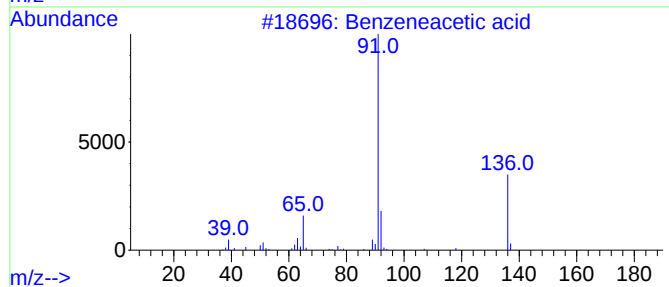
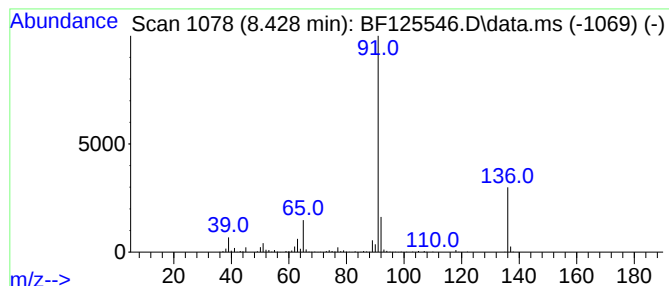
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzeneacetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.428	10.23 ng	849215	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	94
2			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	83
3			Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	72
4			Benzene, (2-methoxyethyl)-	136	C9H12O	003558-60-9	72
5			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
Operator : JU/CG
Sample : M3835-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-CB-04-(1.0)

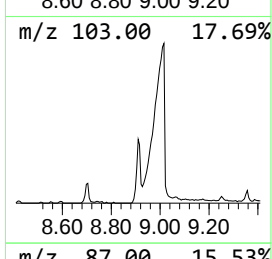
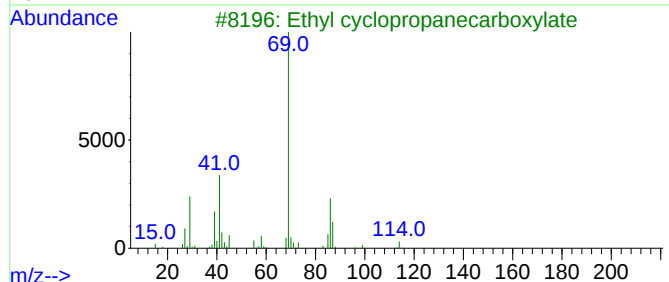
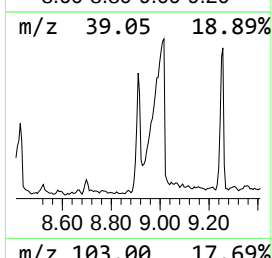
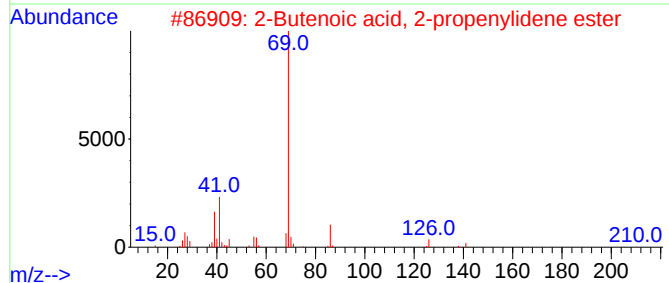
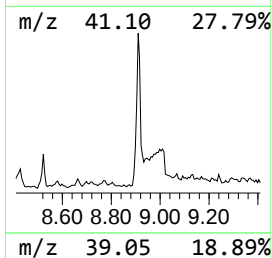
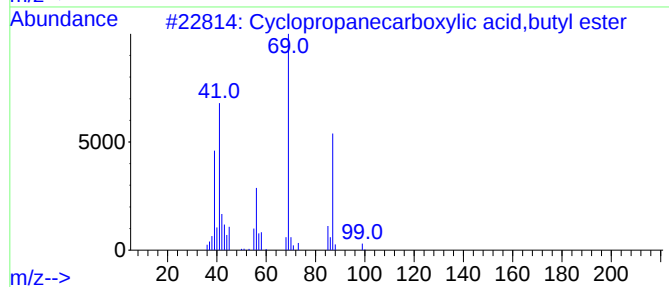
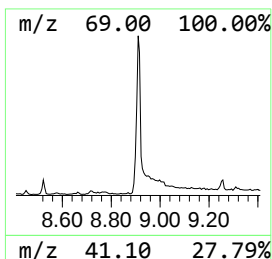
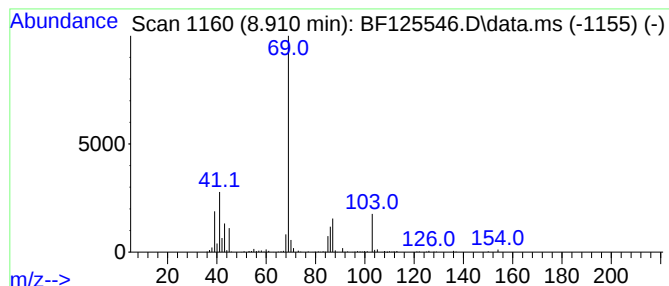
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclopropanecarboxylic acid... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.910	5.00 ng	415026	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	64
2			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
3			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
4			Crotonic anhydride	154	C8H10O3	000623-68-7	38
5			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
Operator : JU/CG
Sample : M3835-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-CB-04-(1.0)

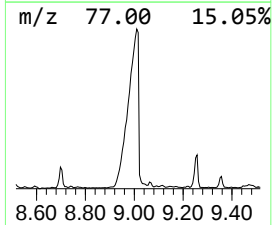
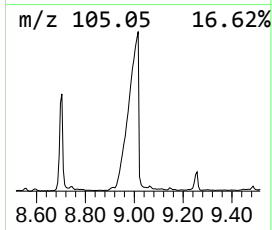
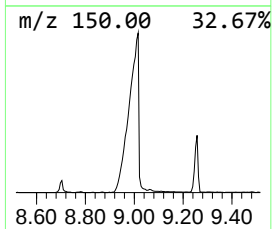
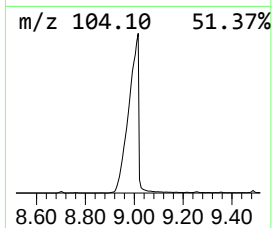
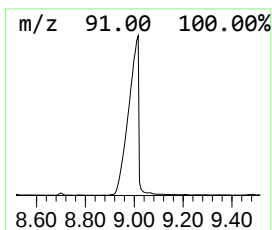
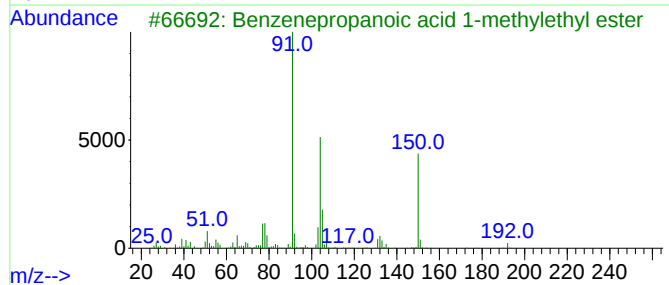
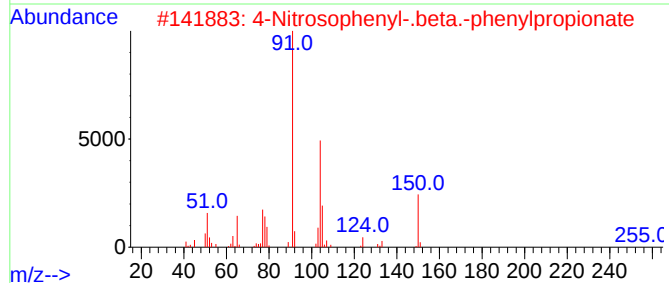
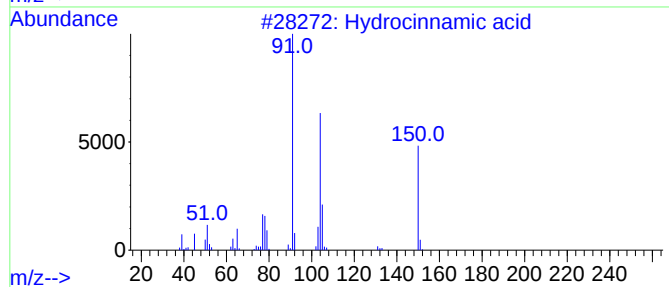
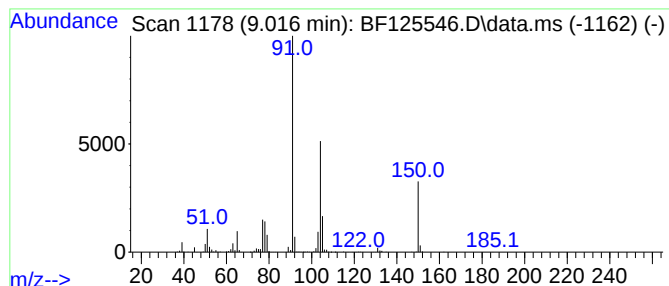
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hydrocinnamic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.016	65.60 ng	5447800	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrocinnamic acid	150	C9H10O2	000501-52-0	97
2			4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	83
3			Benzenepropanoic acid 1-methylet...	192	C12H16O2	022767-95-9	72
4			Benzenepropanoic acid, silver(1+...	256	C9H9AgO2	075112-79-7	53
5			Acetic acid, trifluoro-, 2-pheny...	218	C10H9F3O2	055419-66-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
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Sample : M3835-03
Misc :
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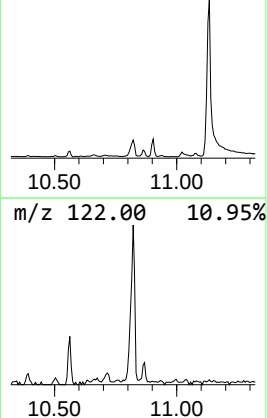
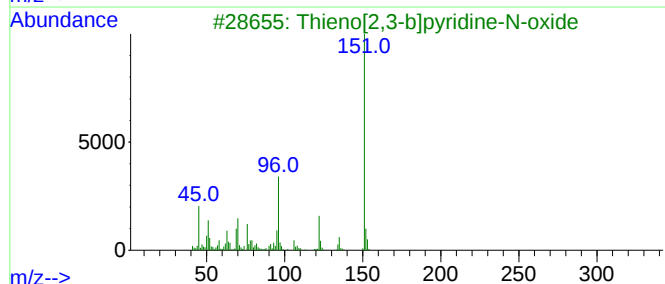
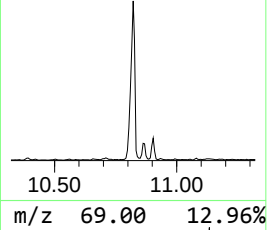
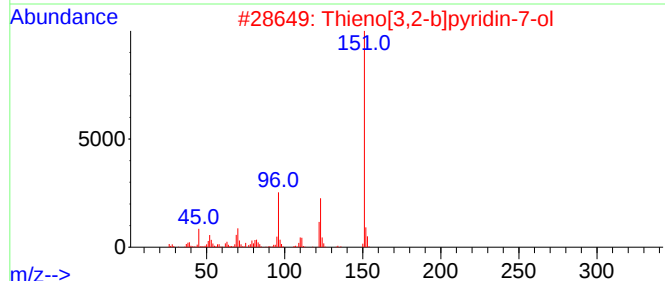
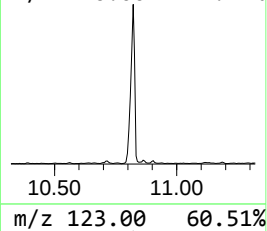
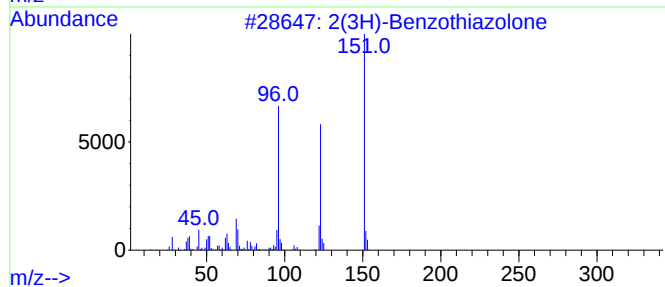
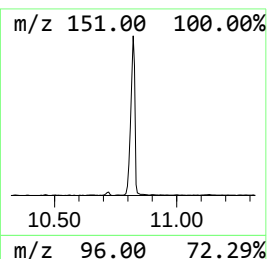
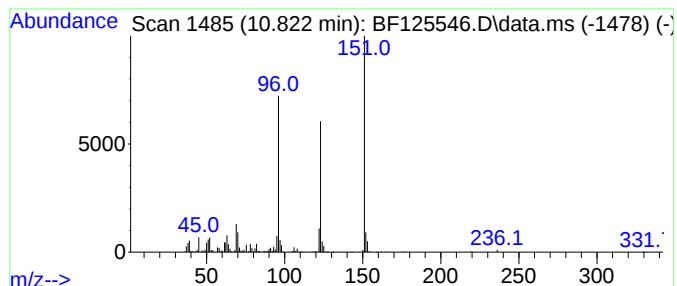
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ClientSampleId :
SW-CB-04-(1.0)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2(3H)-Benzothiazolone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	12.13 ng	1071360	Phenanthrene-d10	11.416
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		2(3H)-Benzothiazolone	151 C7H5NOS	000934-34-9 96
2		Thieno[3,2-b]pyridin-7-ol	151 C7H5NOS	107818-20-2 59
3		Thieno[2,3-b]pyridine-N-oxide	151 C7H5NOS	025557-50-0 53
4		6-Methyl-7-oxo-4,7-dihydro-triaz...	151 C5H5N5O	057250-39-2 50
5		1,2,4-Triazolo[4,3-a]pyridine-3(...	151 C6H5N3S	006952-68-7 38



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Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
Operator : JU/CG
Sample : M3835-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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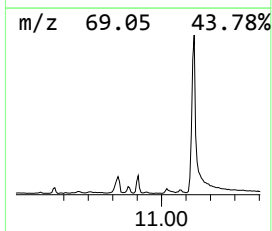
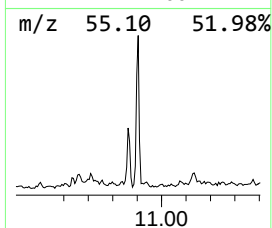
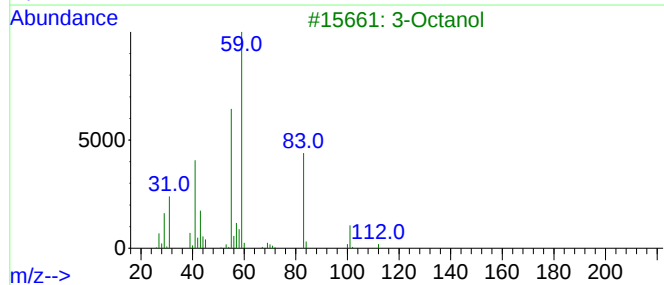
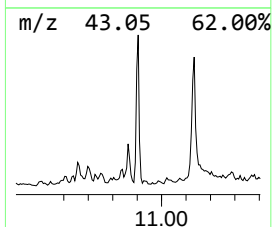
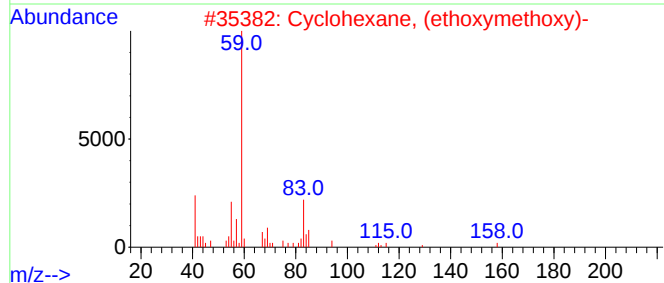
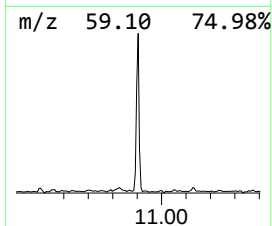
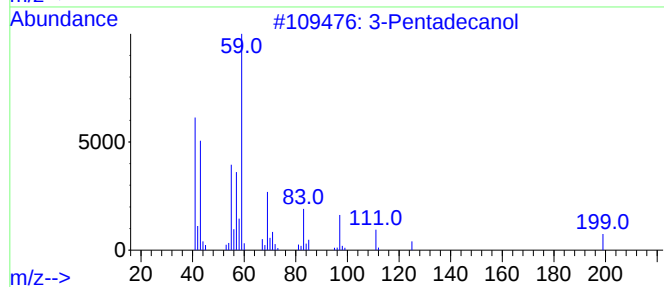
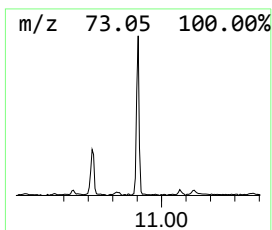
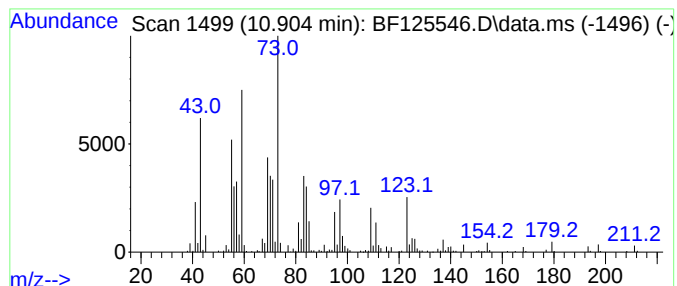
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown10.904 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.904	4.97 ng	438901	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentadecanol	228	C15H32O	053346-71-7	43
2			Cyclohexane, (ethoxymethoxy)-	158	C9H18O2	054699-29-5	38
3			3-Octanol	130	C8H18O	000589-98-0	35
4			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	35
5			Bromoacetic acid, tridecyl ester	320	C15H29BrO2	1000281-85-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
Operator : JU/CG
Sample : M3835-03
Misc :
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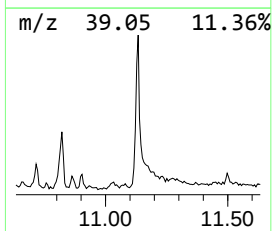
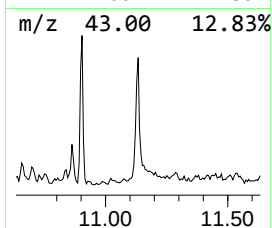
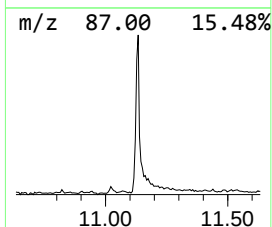
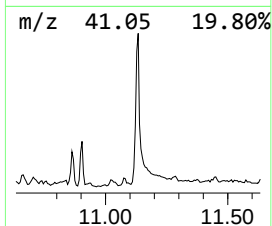
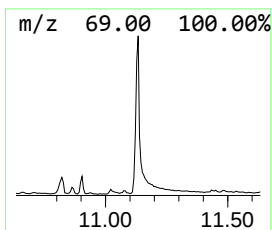
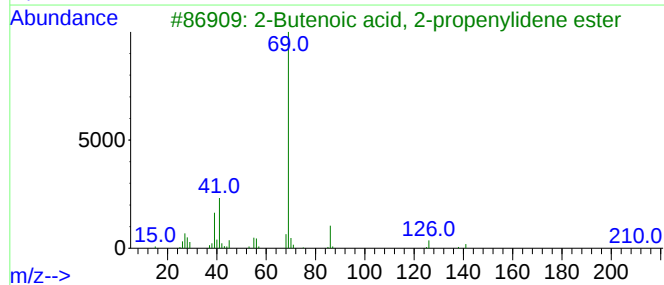
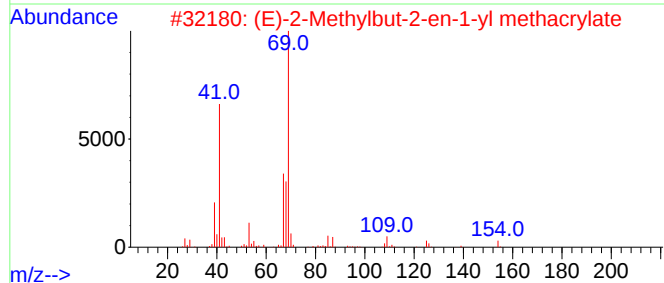
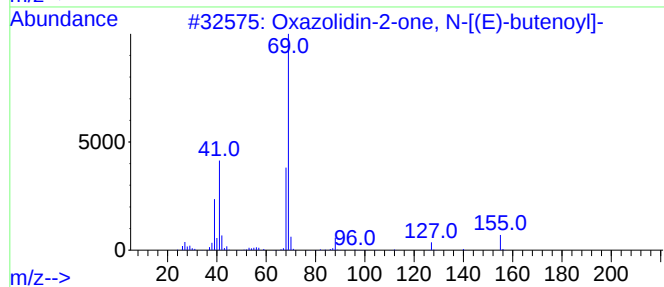
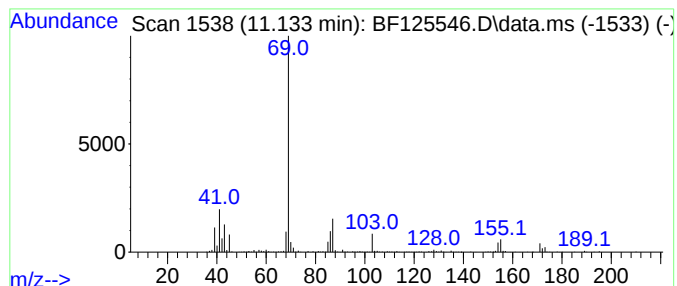
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown11.133 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.133	10.43 ng	921342	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1010156-45-5	47
2			(E)-2-Methylbut-2-en-1-yl methac...	154	C9H14O2	088142-95-4	42
3			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	36
4			2,3'-Bifuran, 2,2',3',5-tetrahydro-	138	C8H10O2	098869-93-3	28
5			3,3,7-Trimethyl-4-oxa-7-octen-1-ol	172	C10H20O2	069161-47-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
Operator : JU/CG
Sample : M3835-03
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ALS Vial : 20 Sample Multiplier: 1

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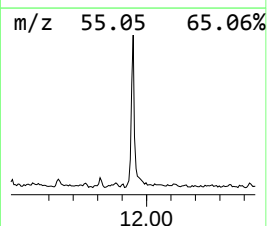
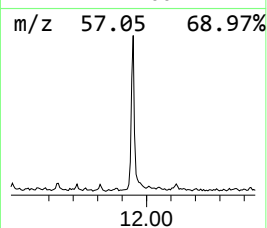
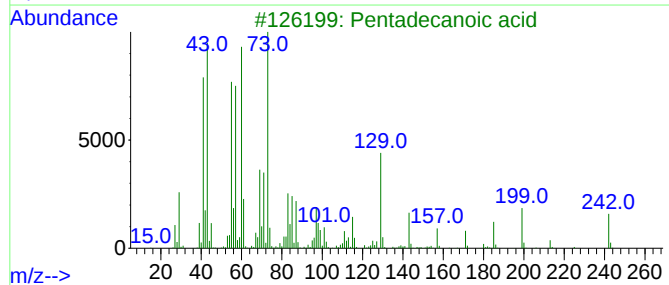
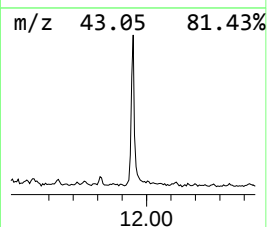
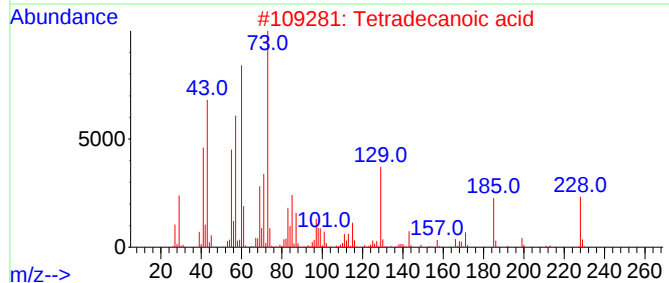
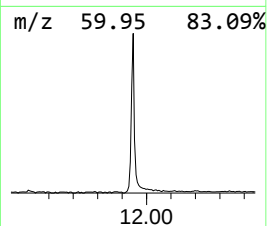
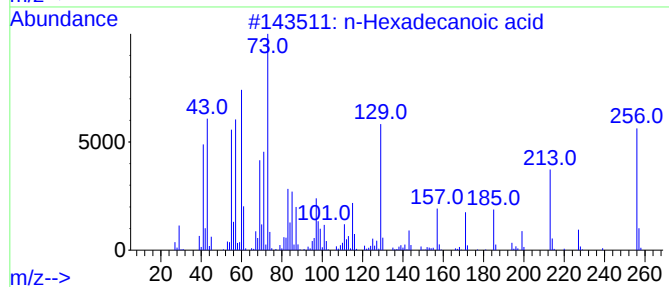
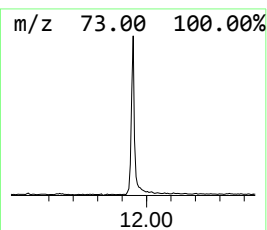
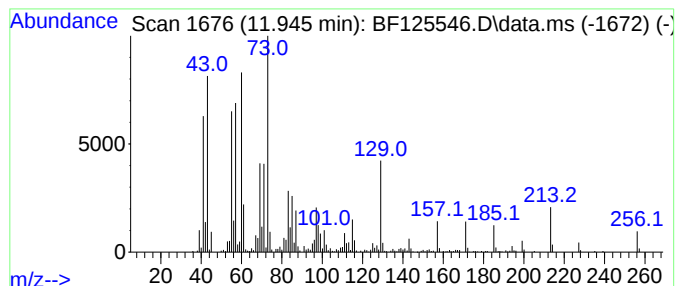
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	7.97 ng	703933	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Undecanoic acid	186	C11H22O2	000112-37-8	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
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Sample : M3835-03
Misc :
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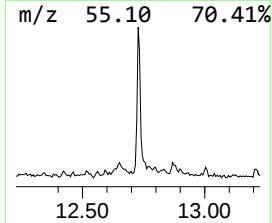
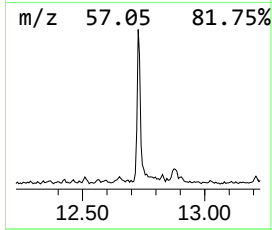
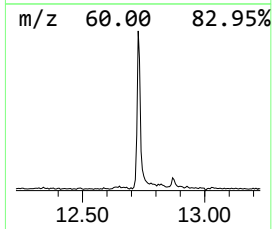
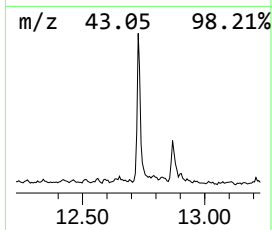
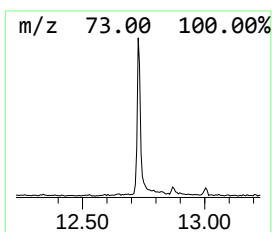
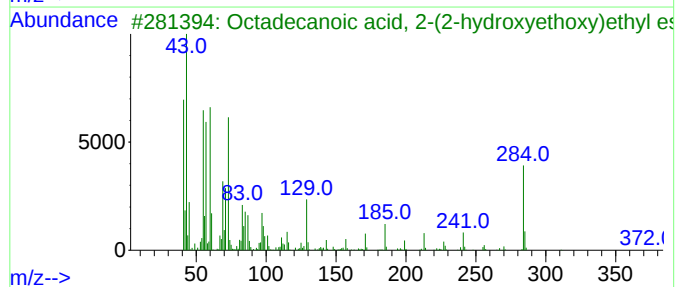
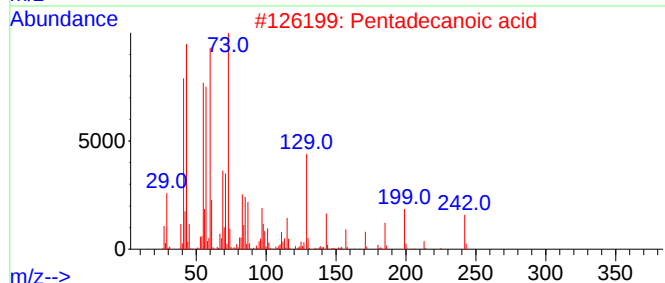
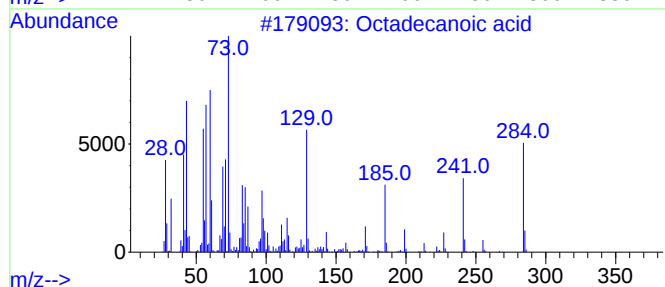
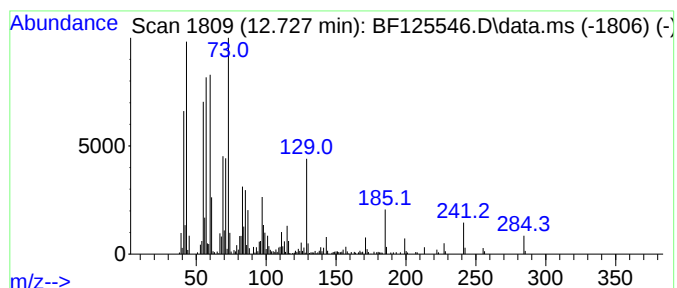
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.727	7.06 ng	623288	Phenanthrene-d10	11.416	
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	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
Operator : JU/CG
Sample : M3835-03
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Instrument :
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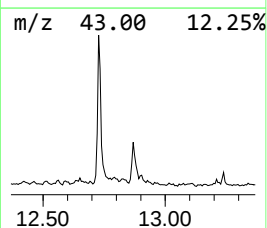
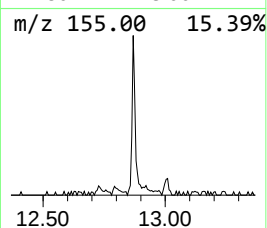
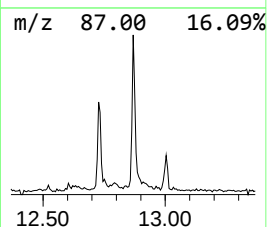
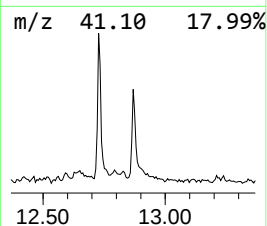
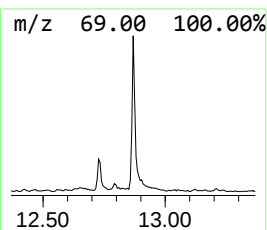
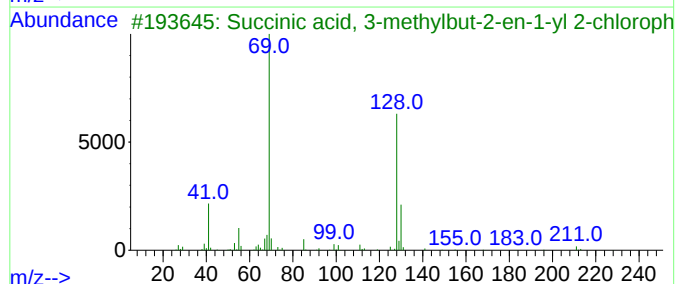
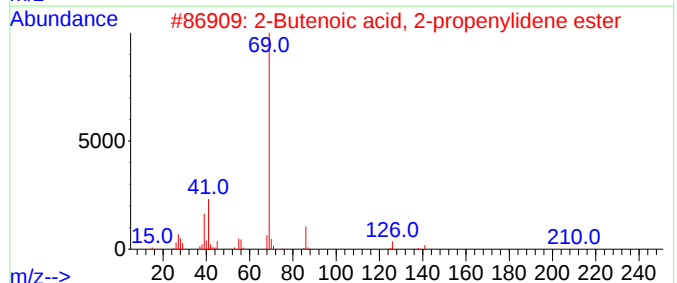
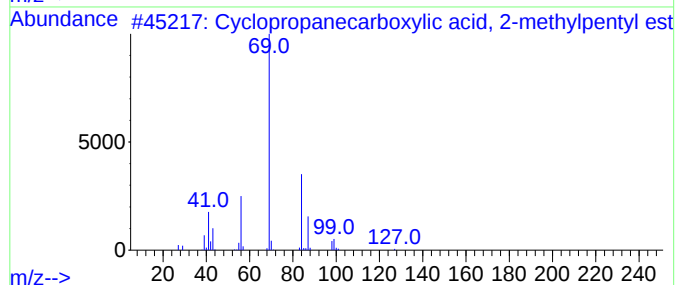
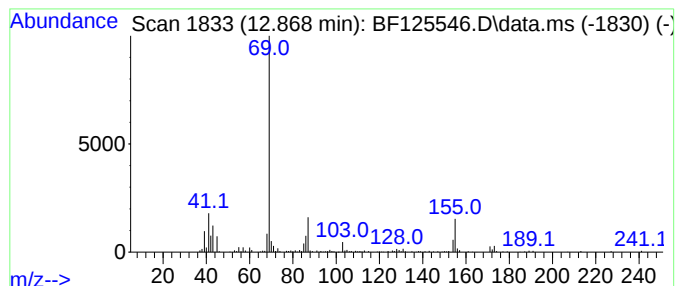
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown12.868 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.868	5.02 ng	294812	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, 2-m...	170	C10H18O2	1000354-65-8	36
2			2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	33
3			Succinic acid, 3-methylbut-2-en-...	296	C15H17ClO4	1000389-79-8	33
4			2,4-Dinitrophenyl crotonate	252	C10H8N2O6	069817-88-5	28
5			Dinocap	207	C10H9NO4	039300-45-3	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
Acq On : 21 Sep 2021 20:44
Operator : JU/CG
Sample : M3835-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

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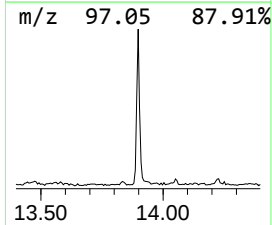
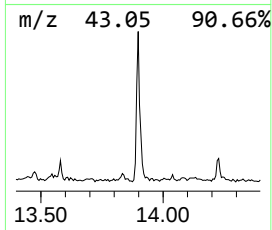
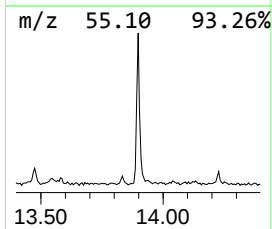
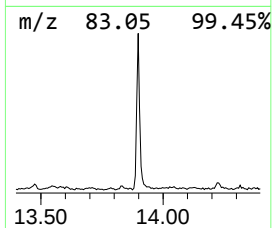
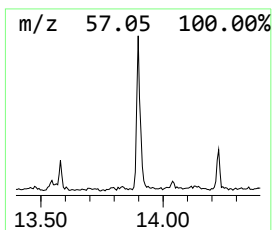
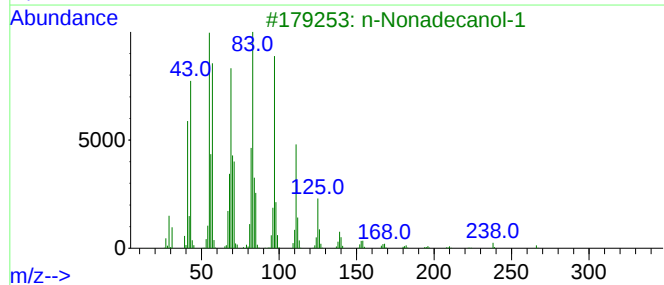
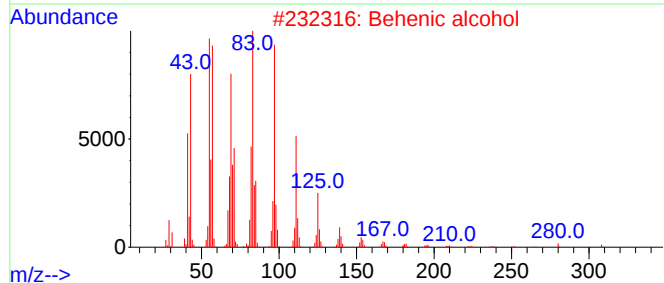
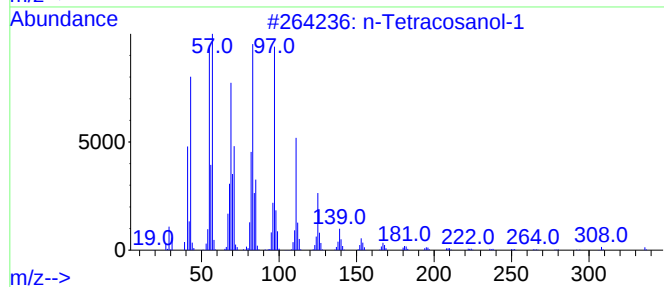
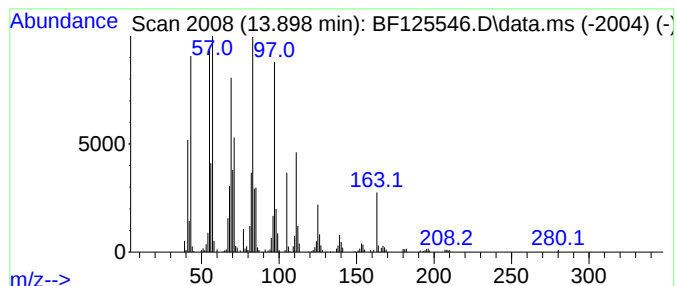
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 n-Tetracosanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	9.12 ng	536133	Chrysene-d12	14.051

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4		1-Hexacosene	364	C26H52	018835-33-1	93
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
Data File : BF125546.D
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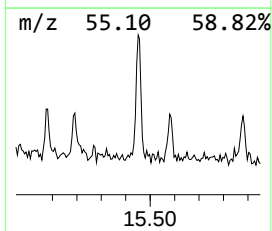
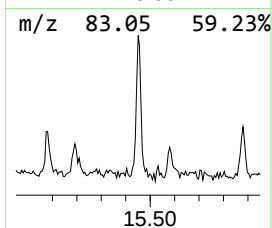
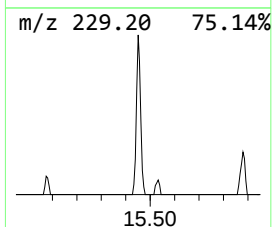
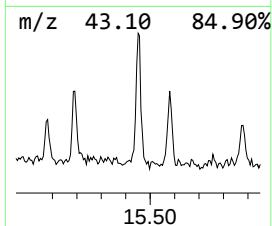
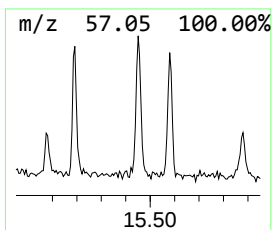
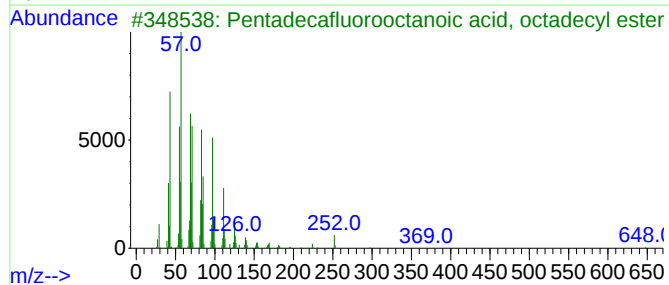
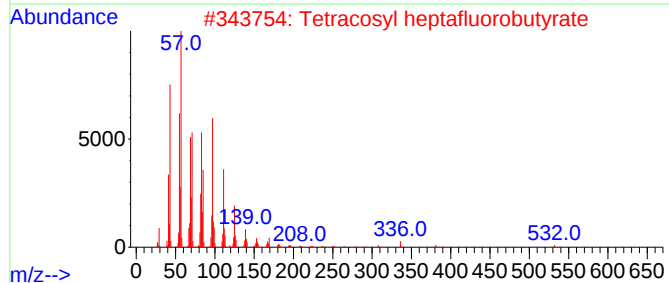
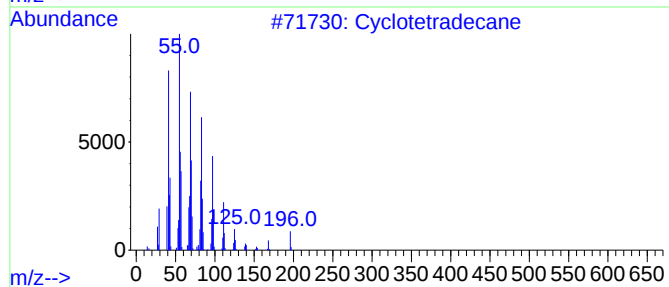
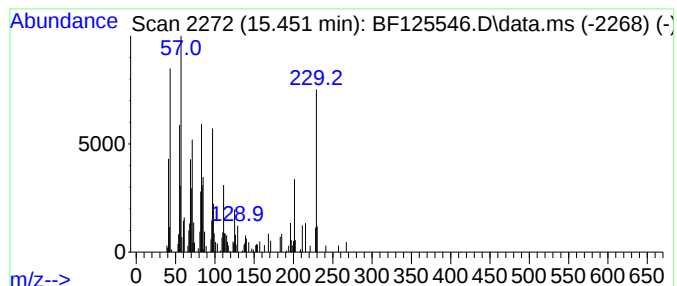
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Cyclotetradecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.451	3.35 ng	190460	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	83
2			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	83
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	53
4			Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	46
5			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092121\
 Data File : BF125546.D
 Acq On : 21 Sep 2021 20:44
 Operator : JU/CG
 Sample : M3835-03
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-CB-04-(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\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.204	68.9	ng	4250900	1	6.898	1234270	20.0
unknown5.110	5.110	3.8	ng	232502	1	6.898	1234270	20.0
Pentanoic acid,...	6.175	3.4	ng	212131	1	6.898	1234270	20.0
Cyclohexanecarb...	7.628	5.8	ng	479319	2	8.181	1660790	20.0
unknown7.722	7.722	31.9	ng	2650350	2	8.181	1660790	20.0
Phenol, 3-ethyl-	7.945	87.7	ng	7280550	2	8.181	1660790	20.0
Ethanol, 2-(2-b...	8.081	9.4	ng	781704	2	8.181	1660790	20.0
Benzeneacetic acid	8.428	10.2	ng	849215	2	8.181	1660790	20.0
Cyclopropanecar...	8.910	5.0	ng	415026	2	8.181	1660790	20.0
Hydrocinnamic acid	9.016	65.6	ng	5447800	2	8.181	1660790	20.0
2(3H)-Benzothia...	10.822	12.1	ng	1071360	4	11.416	1766450	20.0
unknown10.904	10.904	5.0	ng	438901	4	11.416	1766450	20.0
unknown11.133	11.133	10.4	ng	921342	4	11.416	1766450	20.0
n-Hexadecanoic ...	11.945	8.0	ng	703933	4	11.416	1766450	20.0
Octadecanoic acid	12.727	7.1	ng	623288	4	11.416	1766450	20.0
unknown12.868	12.868	5.0	ng	294812	5	14.051	1175360	20.0
n-Tetracosanol-1	13.898	9.1	ng	536133	5	14.051	1175360	20.0
Cyclotetradecane	15.451	3.4	ng	190460	6	15.533	1135770	20.0