

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
 Data File : BF131576.D
 Acq On : 09 Dec 2022 20:17
 Operator : CG\JU
 Sample : N5912-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FMC-TOTE-1207

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-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131576.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	12	18	23	rVB	1323904	1652276	3.07%	0.671%
2	5.304	541	547	549	rBV2	511061	950971	1.77%	0.386%
3	5.628	598	602	609	rBV	301921	540730	1.00%	0.220%
4	5.922	635	652	653	rBV	2619213	6842014	12.71%	2.781%
5	6.069	663	677	680	rVB	321439	1093319	2.03%	0.444%
6	6.286	701	714	716	rBV	4346825	10750750	19.98%	4.369%
7	6.410	729	735	738	rVV	1695520	2311638	4.30%	0.939%
8	7.004	834	836	842	rBV	413579	755202	1.40%	0.307%
9	7.075	844	848	854	rVB3	1444329	1653427	3.07%	0.672%
10	7.322	884	890	897	rBV3	216689	578268	1.07%	0.235%
11	7.481	908	917	920	rBV	1159274	1538837	2.86%	0.625%
12	7.545	925	928	934	rBV2	374759	605860	1.13%	0.246%
13	7.680	942	951	958	rVB	795117	2542444	4.72%	1.033%
14	7.780	958	968	969	rBV4	486313	1103222	2.05%	0.448%
15	7.957	992	998	1002	rVB4	1452575	2121097	3.94%	0.862%
16	8.033	1007	1011	1014	rBV2	542471	614066	1.14%	0.250%
17	8.133	1015	1028	1030	rBV	947820	2564243	4.76%	1.042%
18	8.392	1042	1072	1074	rVB	4222321	23242170	43.19%	9.446%
19	8.504	1074	1091	1092	rBV	14837959	53816630	100.00%	21.871%
20	8.716	1124	1127	1130	rVB	4611416	3775380	7.02%	1.534%
21	8.857	1142	1151	1152	rBV4	2127078	4747595	8.82%	1.929%
22	8.880	1153	1155	1156	rVB	1412980	1059054	1.97%	0.430%
23	8.933	1161	1164	1168	rVV3	2082944	3933774	7.31%	1.599%
24	8.992	1170	1174	1177	rVB4	1590258	2053121	3.82%	0.834%
25	9.045	1177	1183	1184	rBV2	1243317	2091139	3.89%	0.850%
26	9.116	1189	1195	1201	rVB4	2414664	5286389	9.82%	2.148%
27	9.163	1201	1203	1207	rVB2	739241	690835	1.28%	0.281%
28	9.245	1211	1217	1220	rBV3	773723	1490676	2.77%	0.606%
29	9.310	1221	1228	1231	rVV	3525273	6230715	11.58%	2.532%
30	9.357	1231	1236	1238	rVB3	2717688	4569368	8.49%	1.857%
31	9.439	1247	1250	1251	rBV2	750128	628609	1.17%	0.255%
32	9.486	1255	1258	1261	rBV2	1486512	1986924	3.69%	0.807%
33	9.557	1265	1270	1272	rVV2	2041830	2800644	5.20%	1.138%
34	9.592	1272	1276	1283	rVB2	423678	718361	1.33%	0.292%
35	9.792	1298	1310	1315	rVB	2215489	5087107	9.45%	2.067%
36	9.980	1339	1342	1346	rVB2	695859	684775	1.27%	0.278%

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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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.386	1404	1411	1415	rBV2	1292056	1961658	3.65%	0.797%
38	10.510	1428	1432	1435	rBV2	443901	542936	1.01%	0.221%
39	10.539	1435	1437	1442	rVB	1087596	1066381	1.98%	0.433%
40	10.627	1449	1452	1460	rVB	1860718	2237785	4.16%	0.909%
41	10.721	1465	1468	1473	rVB3	1041084	1175332	2.18%	0.478%
42	10.774	1473	1477	1479	rBV	987357	911112	1.69%	0.370%
43	10.851	1487	1490	1497	rBV	1274016	1568356	2.91%	0.637%
44	11.316	1565	1569	1572	rBV	503071	604715	1.12%	0.246%
45	11.386	1574	1581	1583	rVV	1798199	2301013	4.28%	0.935%
46	11.433	1583	1589	1592	rVV	1767496	1734277	3.22%	0.705%
47	11.527	1602	1605	1608	rVV	1429049	1195347	2.22%	0.486%
48	11.621	1619	1621	1626	rVB	1293854	1276728	2.37%	0.519%
49	11.674	1626	1630	1635	rBV	518795	630183	1.17%	0.256%
50	11.763	1640	1645	1652	rVB	1536147	2021324	3.76%	0.821%
51	11.851	1657	1660	1662	rBV	1676931	1957128	3.64%	0.795%
52	11.933	1671	1674	1679	rVV	1367140	1487617	2.76%	0.605%
53	12.051	1691	1694	1703	rVB	2018467	2251401	4.18%	0.915%
54	12.451	1759	1762	1767	rVB	837828	903942	1.68%	0.367%
55	12.721	1805	1808	1809	rVV	1047733	933559	1.73%	0.379%
56	12.851	1825	1830	1839	rVB	1641298	2514519	4.67%	1.022%
57	12.927	1839	1843	1846	rVV	1791398	2214570	4.12%	0.900%
58	12.957	1846	1848	1853	rVV	1377633	1602237	2.98%	0.651%
59	13.004	1853	1856	1862	rVV	1766695	2018287	3.75%	0.820%
60	13.057	1862	1865	1868	rVB	992173	899575	1.67%	0.366%
61	13.104	1869	1873	1883	rBV	2593259	2982052	5.54%	1.212%
62	13.457	1930	1933	1942	rBV	1172723	1420604	2.64%	0.577%
63	13.698	1971	1974	1978	rVV	994680	1265336	2.35%	0.514%
64	13.733	1978	1980	1987	rVV	432242	678943	1.26%	0.276%
65	13.815	1988	1994	2001	rVV2	1299246	2920426	5.43%	1.187%
66	13.880	2001	2005	2008	rVV	2032174	2350904	4.37%	0.955%
67	13.915	2008	2011	2015	rVV	1723544	2099712	3.90%	0.853%
68	13.957	2015	2018	2028	rVV	2058583	2673364	4.97%	1.086%
69	14.039	2028	2032	2039	rVV	2989977	3558888	6.61%	1.446%
70	14.351	2082	2085	2092	rBV	1320119	1690544	3.14%	0.687%
71	14.568	2119	2122	2125	rBV	881636	1057938	1.97%	0.430%
72	14.674	2134	2140	2144	rBV2	1087604	2350912	4.37%	0.955%
73	14.745	2148	2152	2156	rVV	1749589	2419441	4.50%	0.983%
74	14.786	2156	2159	2162	rVV	1548911	1976467	3.67%	0.803%
75	14.821	2162	2165	2175	rVV	1782734	2387730	4.44%	0.970%
76	14.904	2175	2179	2189	rVV	2476126	3572579	6.64%	1.452%

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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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	15.256	2235	2239	2249	rVB	953910	1546947	2.87%	0.629%
78	15.527	2281	2285	2289	rBV	409957	683892	1.27%	0.278%
79	15.668	2300	2309	2315	rBV2	506726	1695337	3.15%	0.689%
80	15.762	2321	2325	2333	rVB	716559	1247641	2.32%	0.507%
81	15.833	2333	2337	2341	rVV	629340	1167838	2.17%	0.475%
82	15.874	2341	2344	2357	rVB	761594	1524686	2.83%	0.620%
83	15.986	2358	2363	2379	rVB	1064962	2222994	4.13%	0.903%
84	16.492	2443	2449	2461	rVB	277566	712485	1.32%	0.290%
85	17.574	2627	2633	2656	rVB	197745	732966	1.36%	0.298%

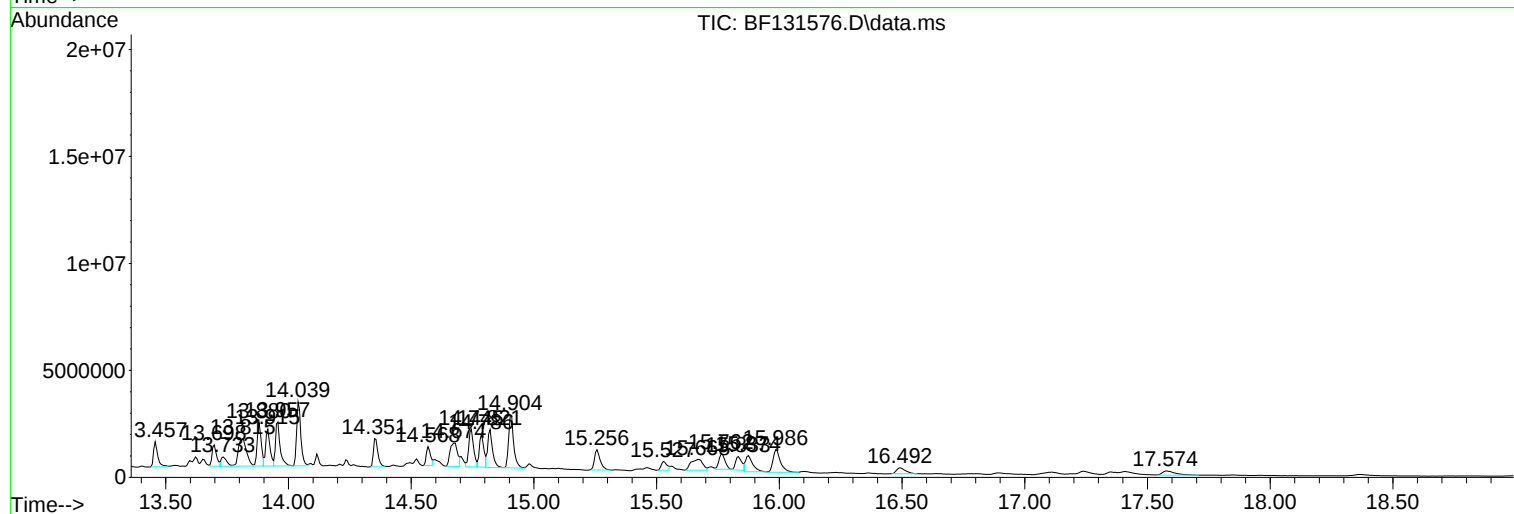
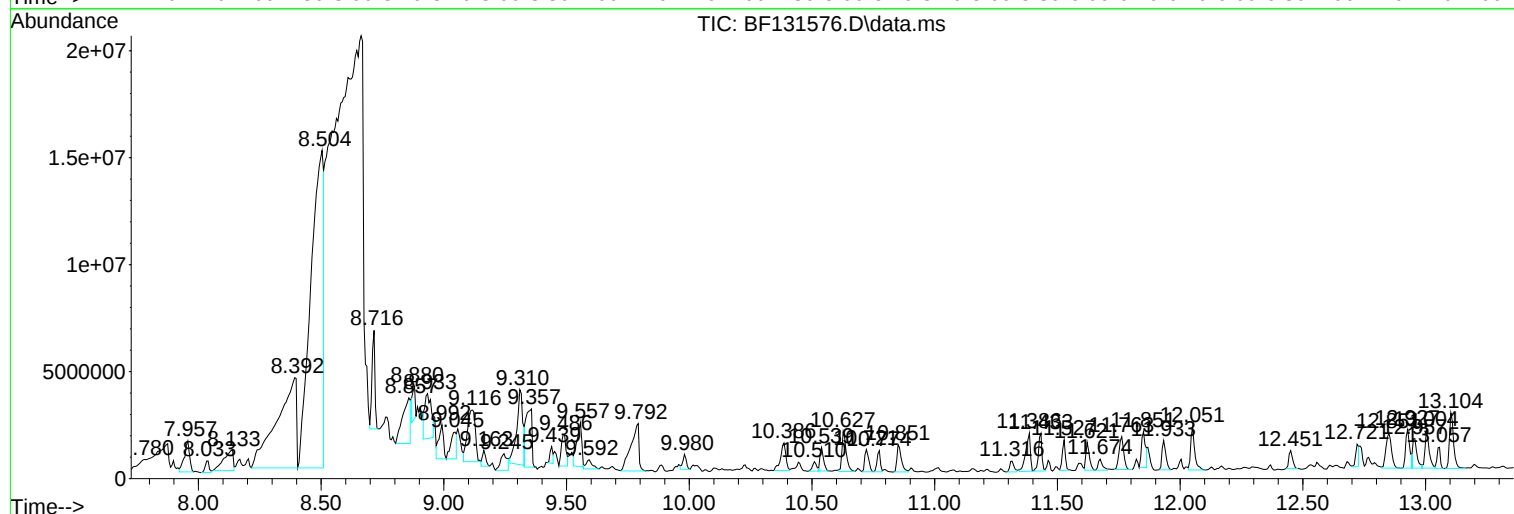
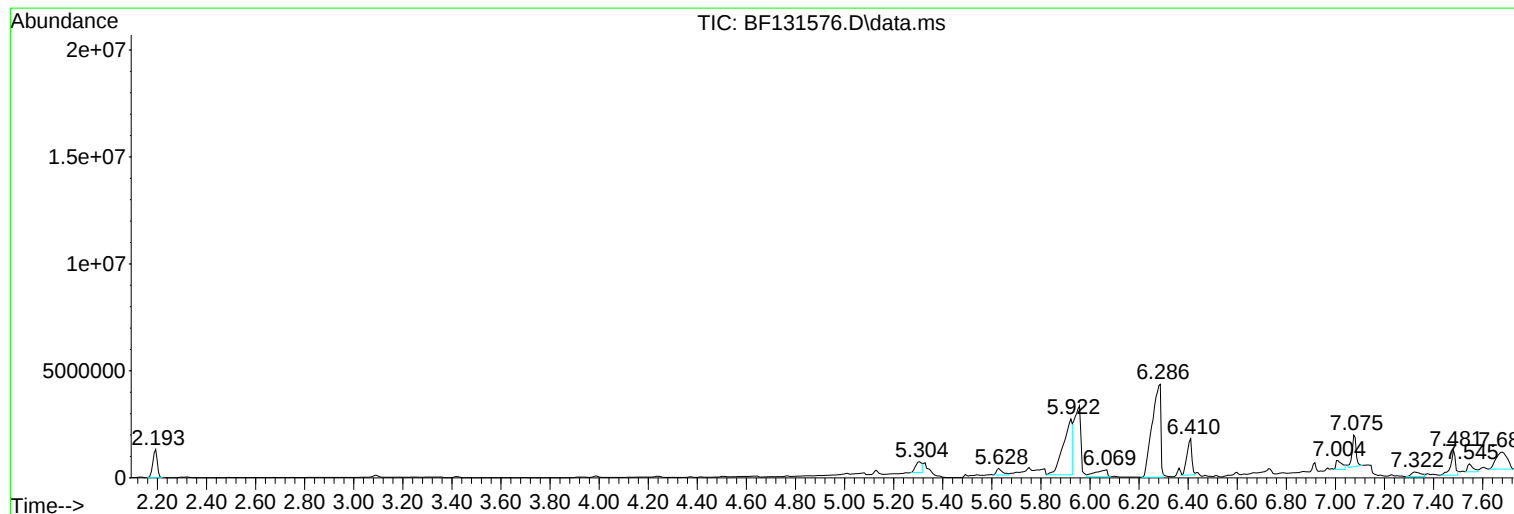
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Instrument :
BNA_F
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FMC-TOTE-1207

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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\BF120922\
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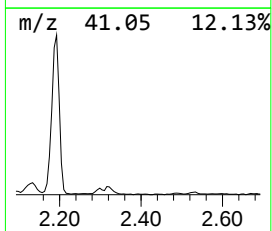
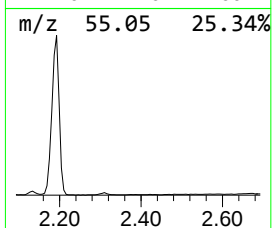
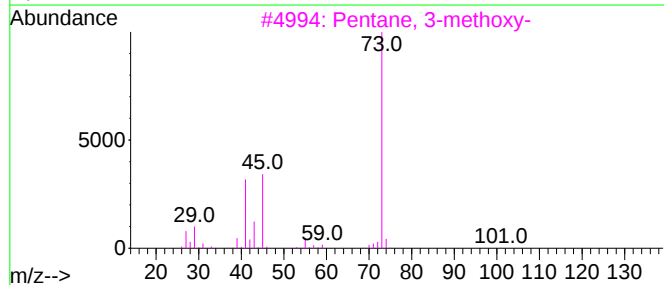
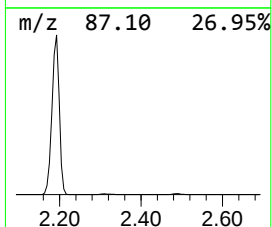
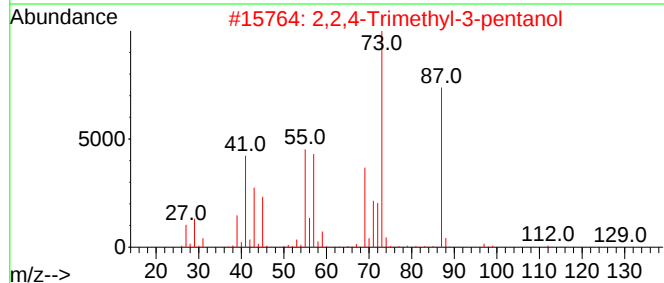
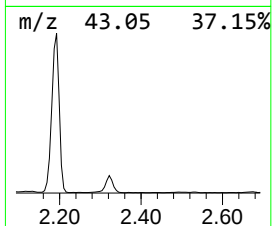
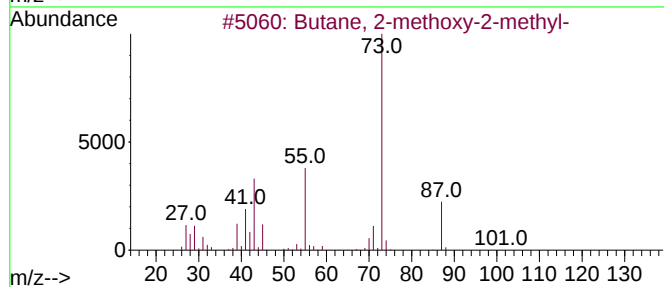
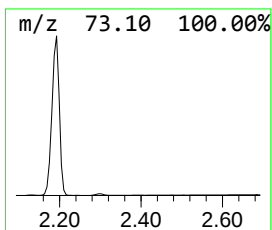
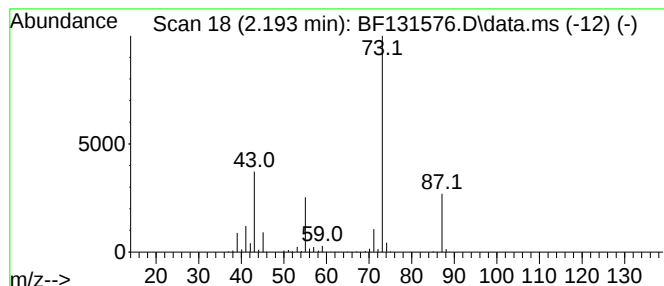
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	43.76 ng	1652280	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			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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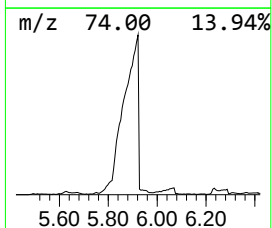
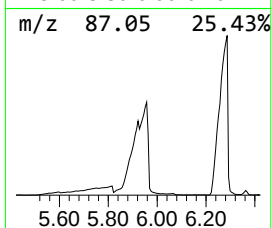
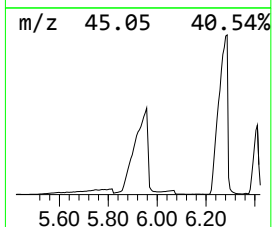
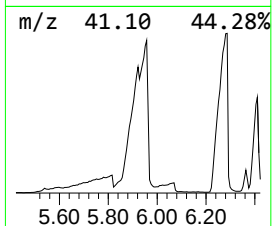
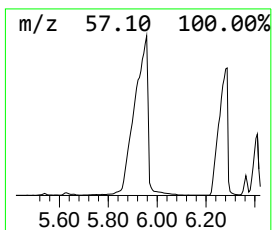
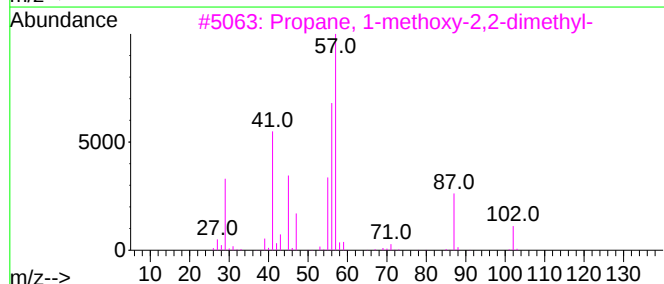
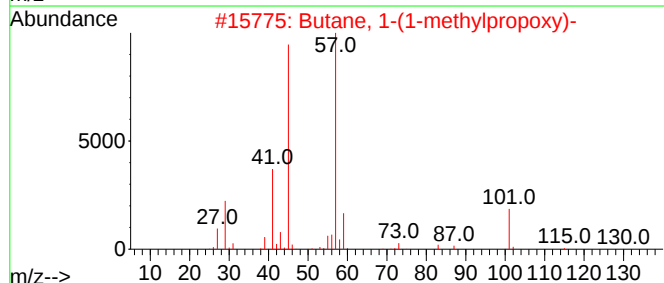
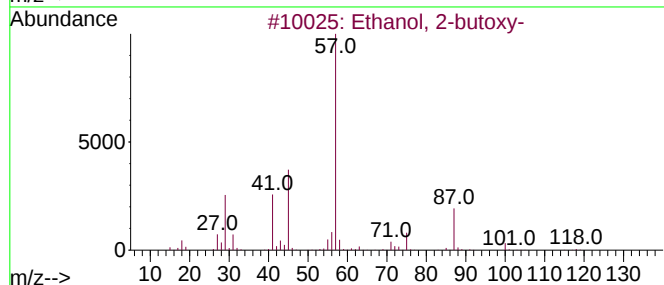
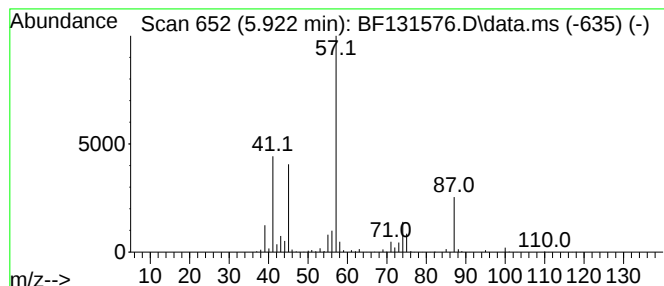
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.922	181.20 ng	6842010	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	64
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3			Propane, 1-methoxy-2,2-dimethyl-	102	C6H14O	001118-00-9	53
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	42
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	40



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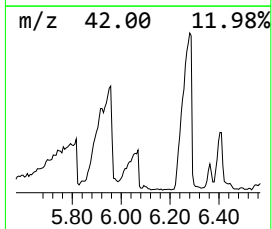
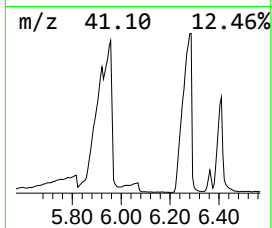
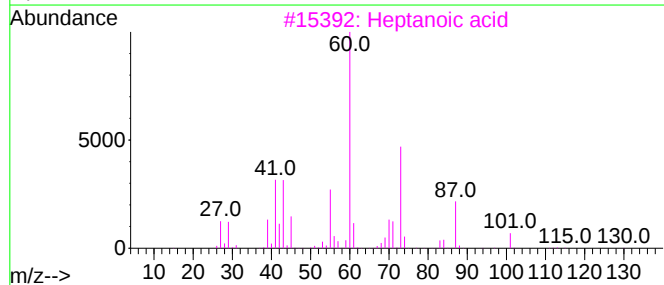
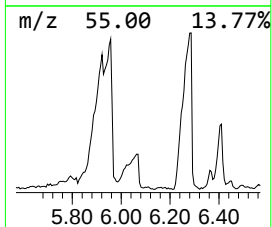
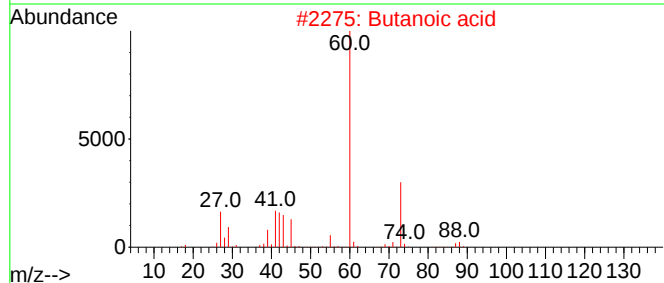
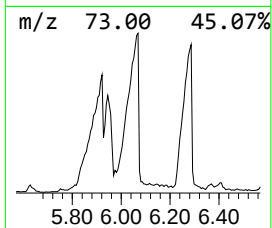
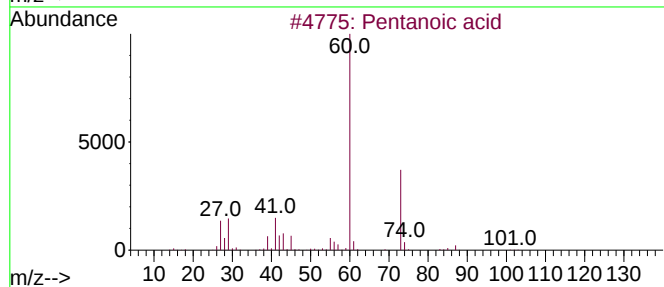
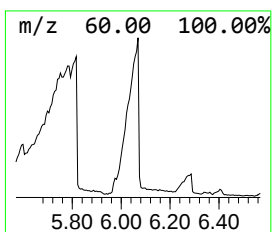
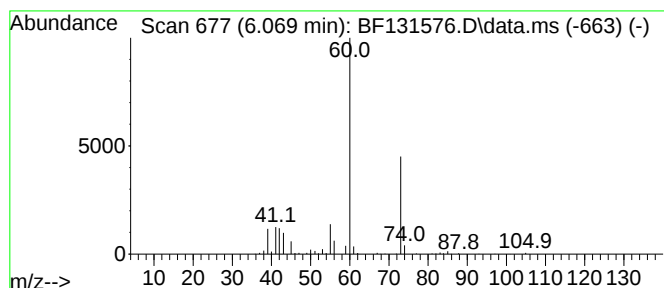
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.069	28.95 ng	1093320	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid	102	C5H10O2	000109-52-4	78
2			Butanoic acid	88	C4H8O2	000107-92-6	64
3			Heptanoic acid	130	C7H14O2	000111-14-8	40
4			Hexanoic acid	116	C6H12O2	000142-62-1	40
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	38



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Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FMC-TOTE-1207

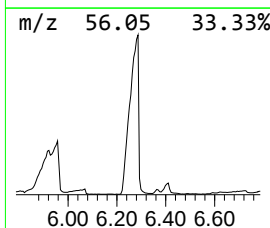
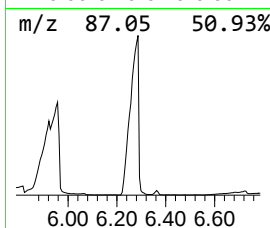
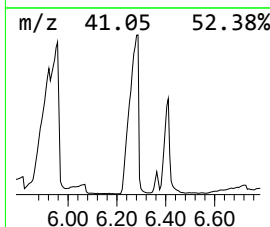
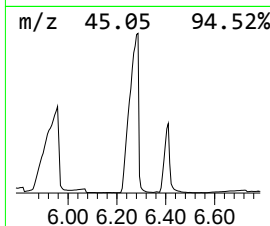
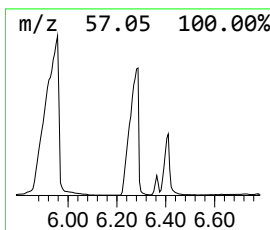
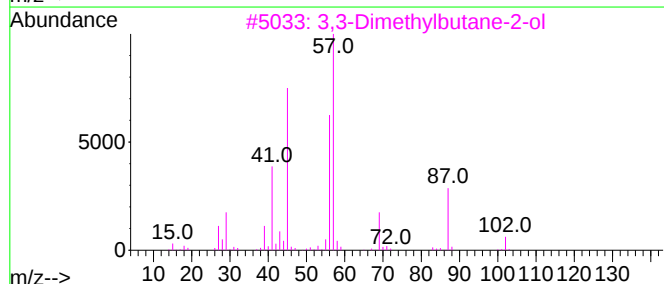
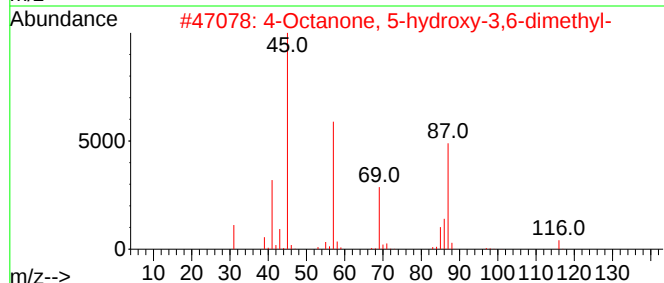
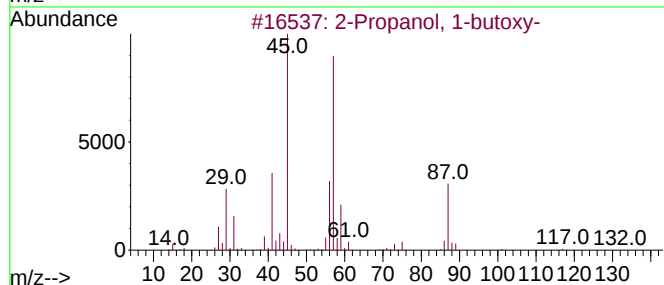
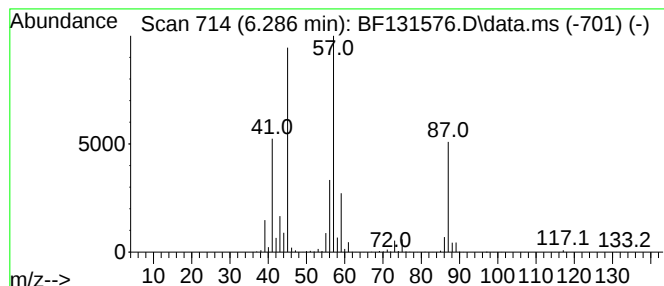
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Propanol, 1-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.286	284.71 ng	10750800	1,4-Dichlorobenzene-d4	6.916

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	78
2		4-Octanone, 5-hydroxy-3,6-dimethyl-	172	C10H20O2	062759-47-1	42
3		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
4		Hexane, 1,2,3-trimethoxy-	176	C9H20O3	020637-29-0	40
5		5-Methyl-1-hepten-4-ol	128	C8H16O	099328-46-8	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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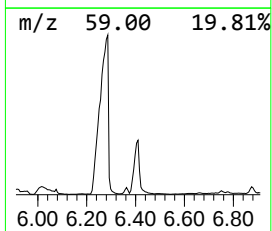
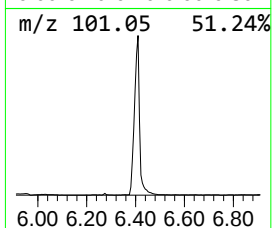
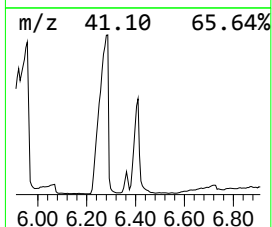
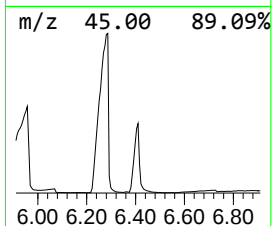
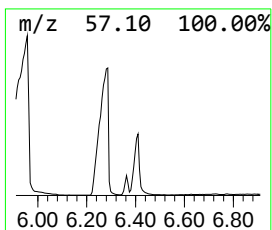
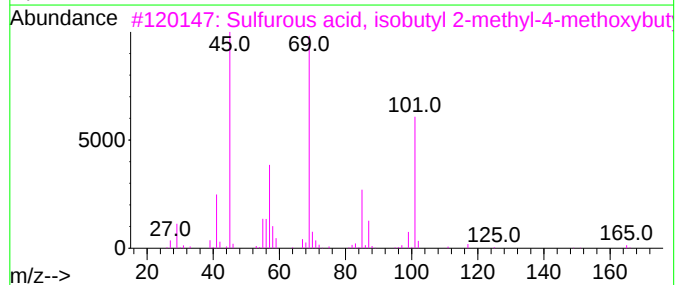
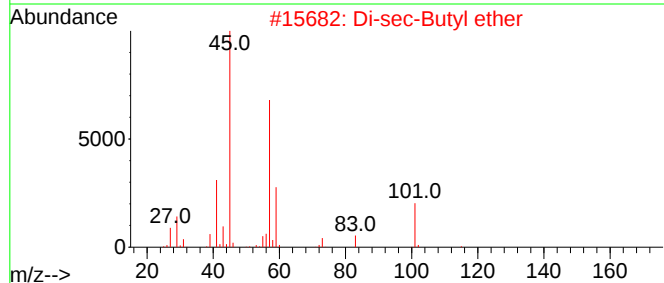
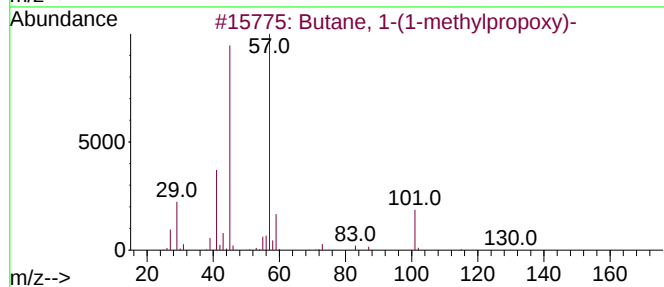
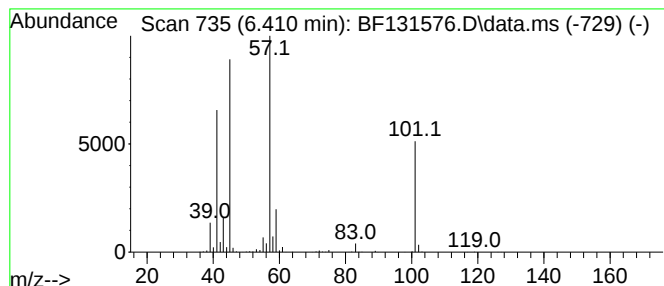
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Butane, 1-(1-methylpropoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.410	61.22 ng	2311640	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	64
2			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
3			Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	38
4			Butane, 2-ethoxy-	102	C6H14O	002679-87-0	38
5			Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FMC-TOTE-1207

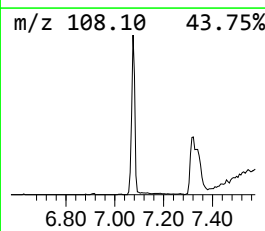
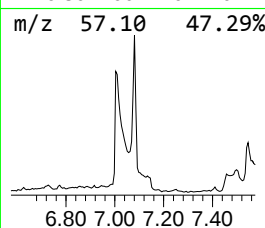
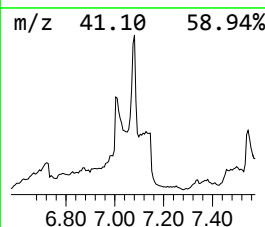
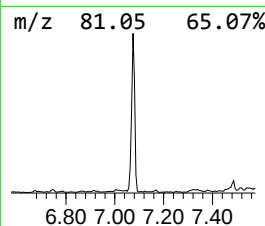
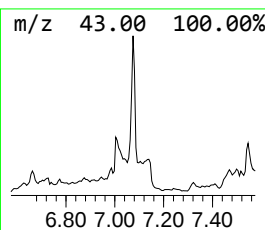
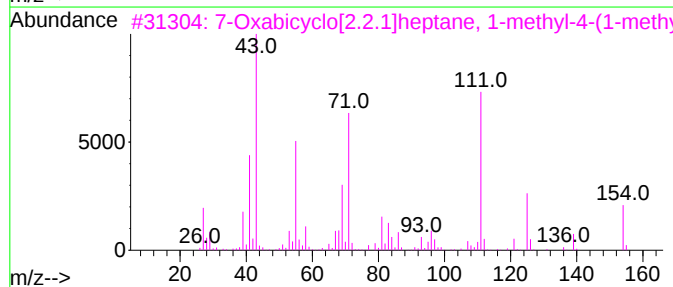
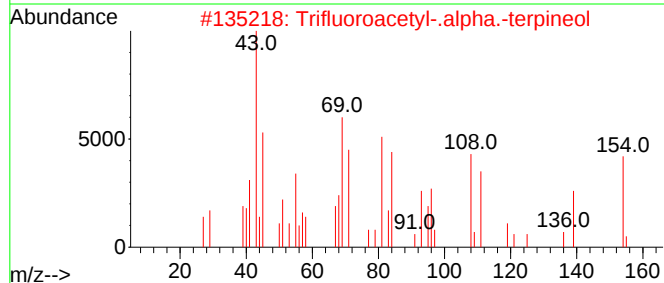
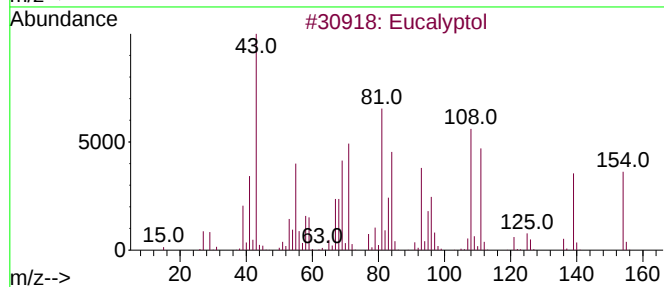
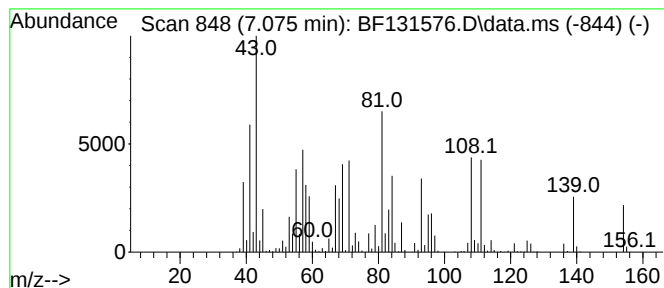
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eucalyptol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.075	43.79 ng	1653430	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	96
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	50
3			7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	35
4			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	25
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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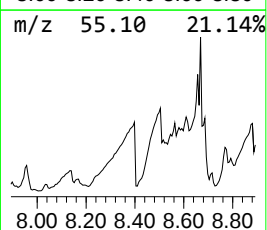
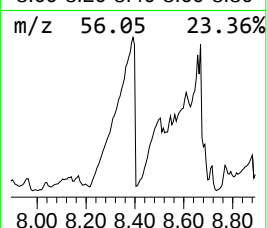
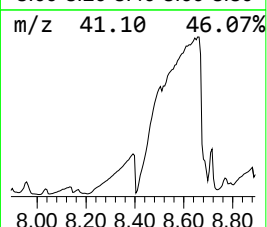
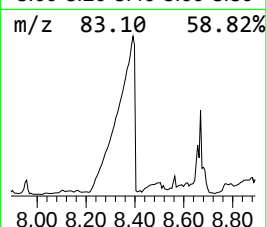
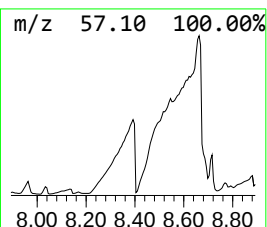
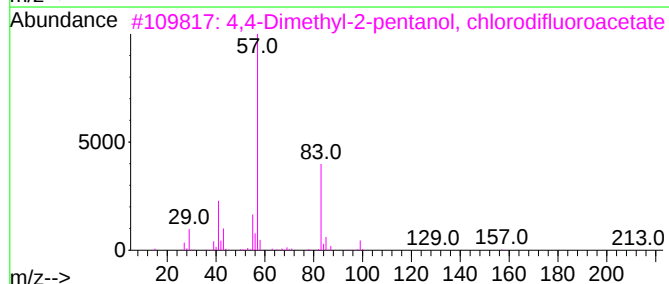
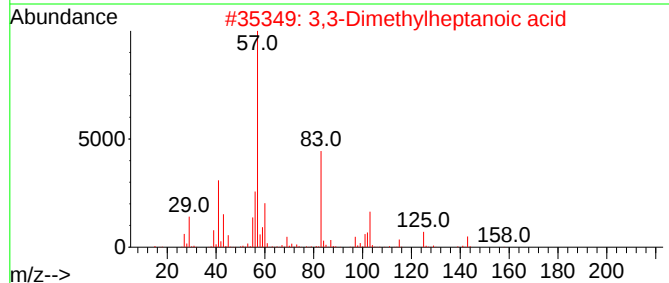
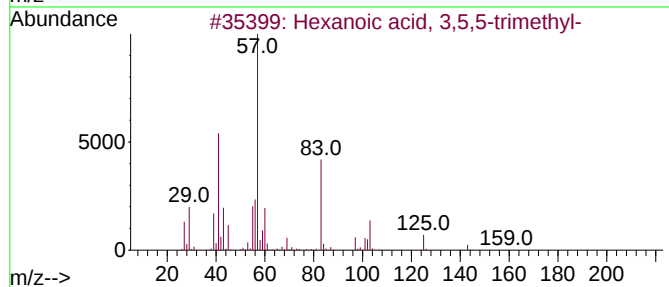
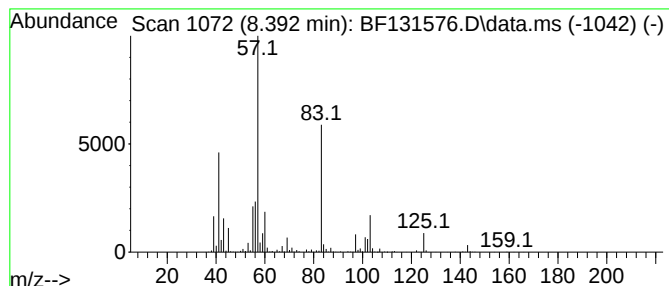
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexanoic acid, 3,5,5-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.392	181.28 ng	23242200	Naphthalene-d8	8.204

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2		3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3		4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	43
4		Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	42
5		6,6-Dimethylheptanoic acid	158	C9H18O2	015898-92-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
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Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

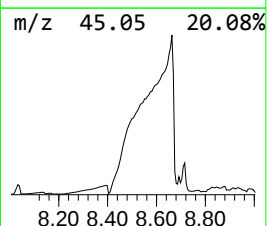
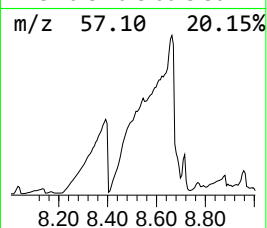
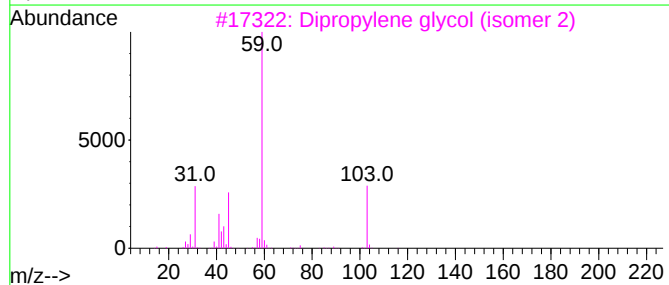
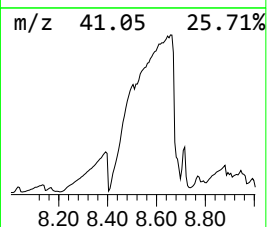
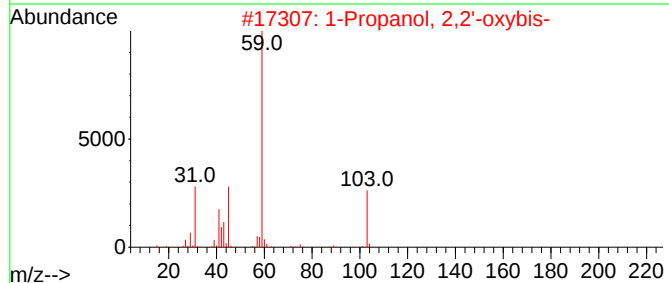
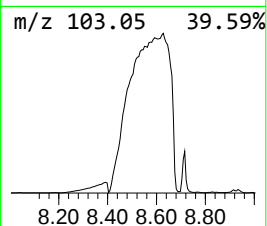
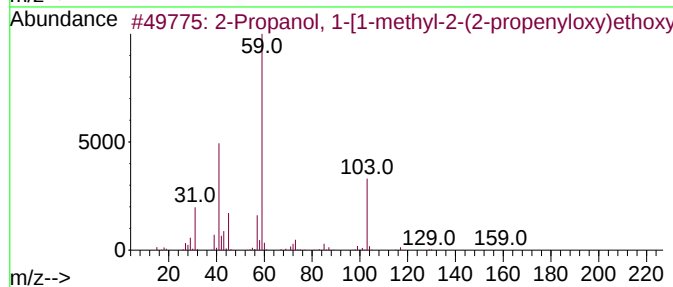
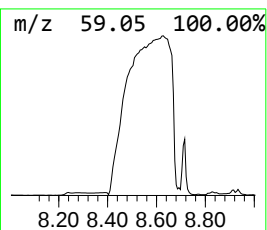
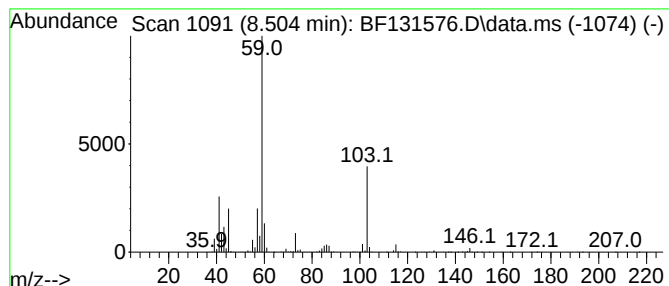
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.504	419.75 ng	53816600	Naphthalene-d8	8.204	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	72
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	64
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
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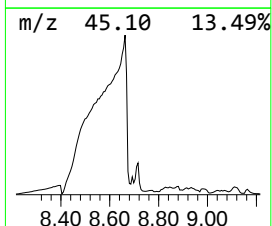
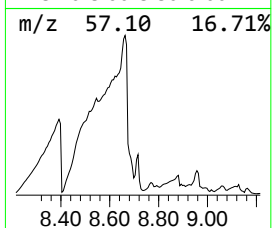
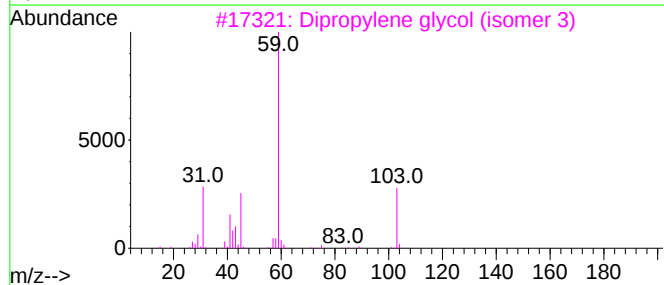
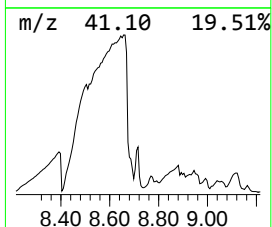
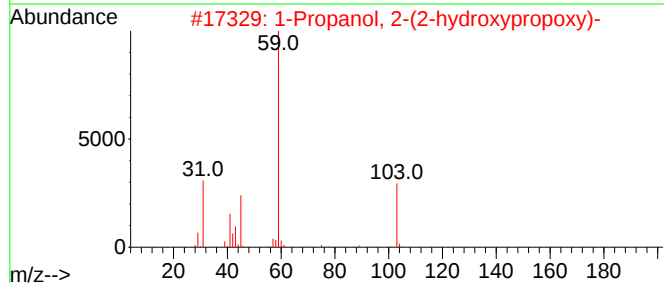
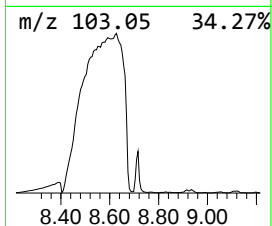
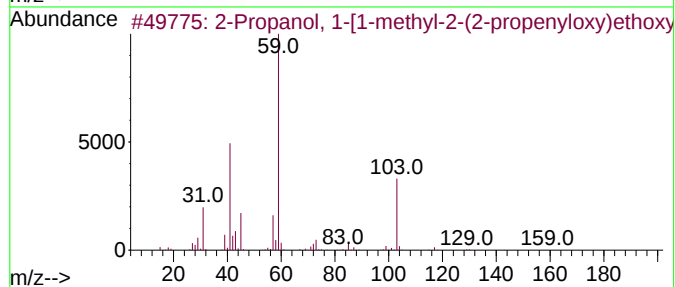
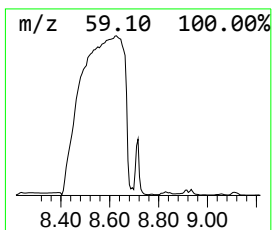
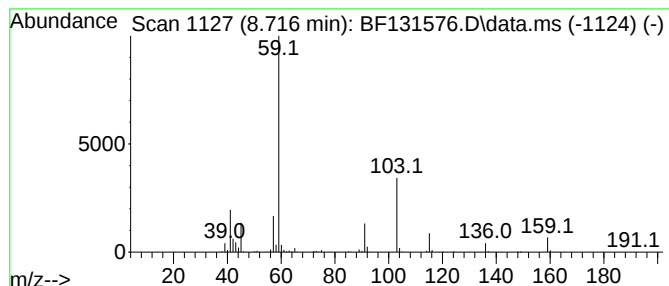
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Propanol, 2-(2-hydroxypro... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.716	29.45 ng	3775380	Naphthalene-d8	8.204	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	64
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59
3	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	59
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	59
5	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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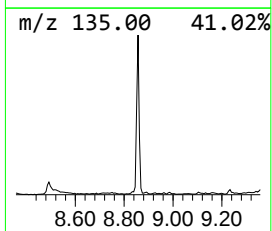
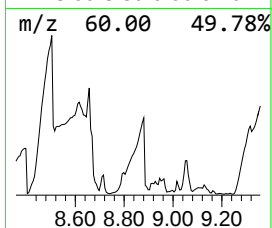
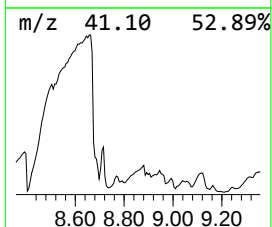
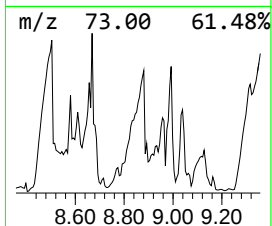
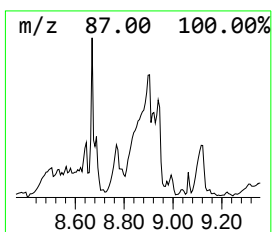
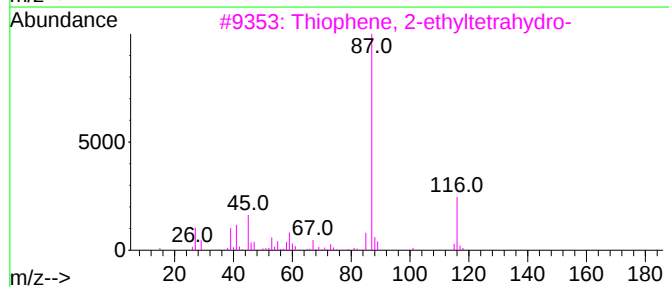
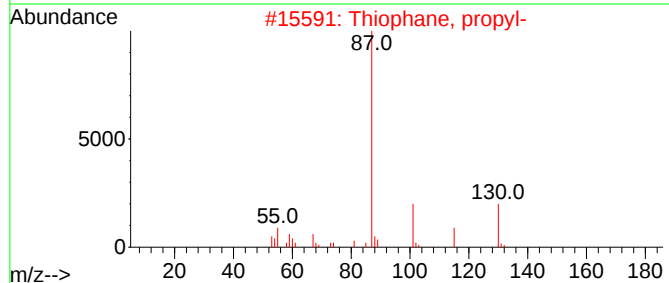
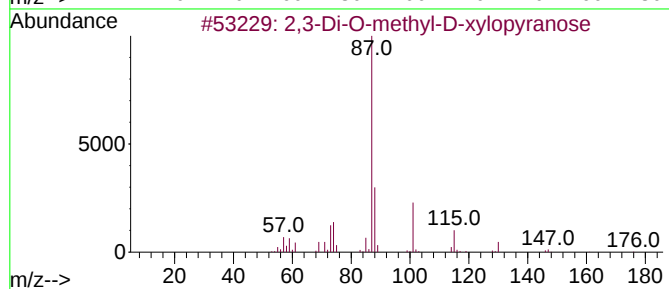
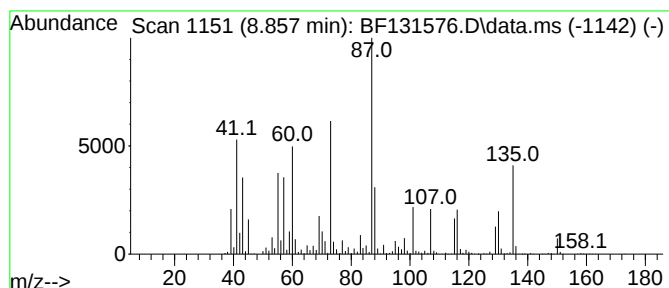
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown8.857 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.857	37.03 ng	4747600	Naphthalene-d8	8.204

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,3-Di-O-methyl-D-xylopyranose	178	C7H14O5	018186-26-0	43
2		Thiophane, propyl-	130	C7H14S	001551-34-4	35
3		Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	30
4		Pivaloin	172	C10H20O2	000815-66-7	25
5		3-Methylundecanoic acid	200	C12H24O2	065781-38-6	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FMC-TOTE-1207

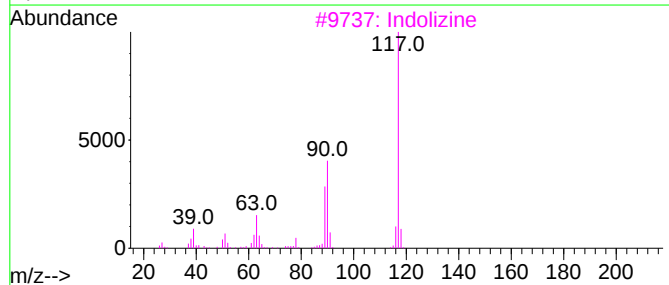
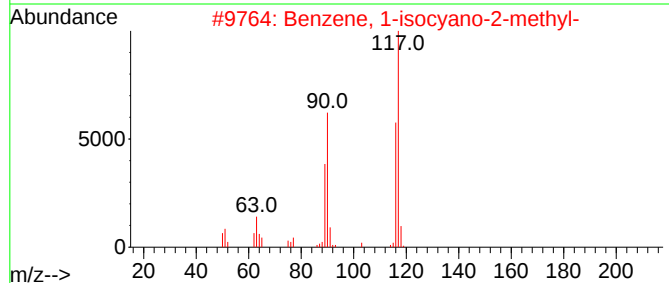
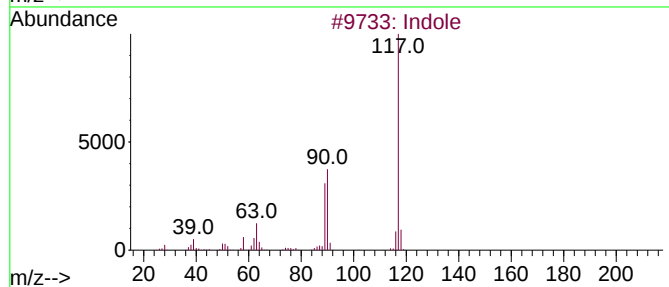
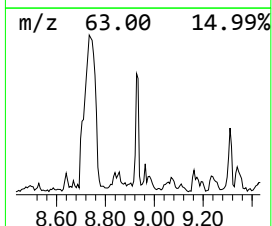
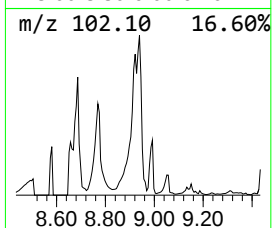
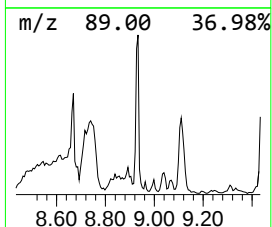
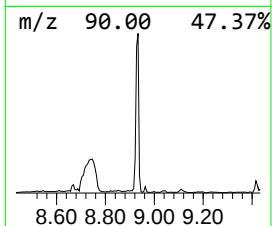
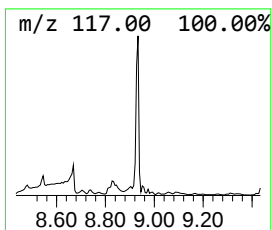
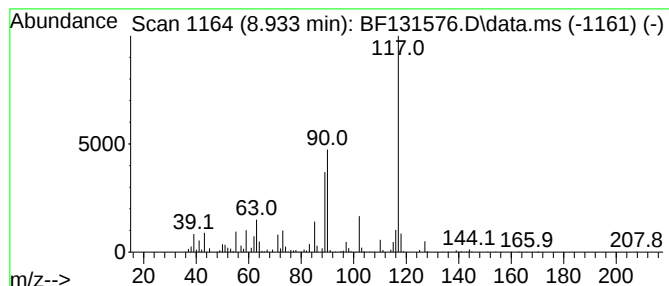
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Indole Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.933	30.68 ng	3933770	Naphthalene-d8	8.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	94
2			Benzene, 1-isocyano-2-methyl-	117	C8H7N	010468-64-1	70
3			Indolizine	117	C8H7N	000274-40-8	68
4			5H-1-Pyridine	117	C8H7N	000270-91-7	68
5			Benzyl nitrile	117	C8H7N	000140-29-4	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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ClientSampleId :
FMC-TOTE-1207

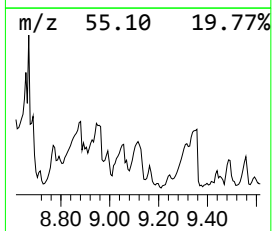
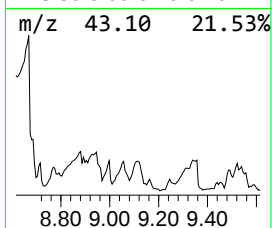
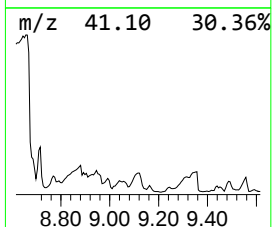
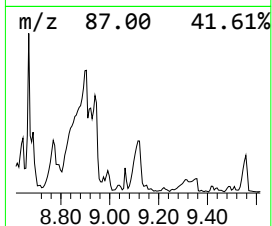
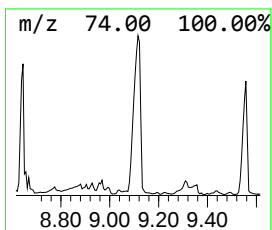
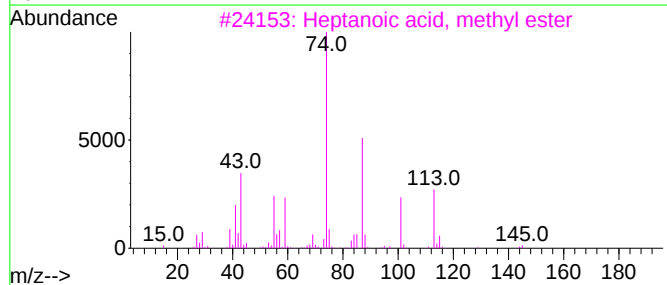
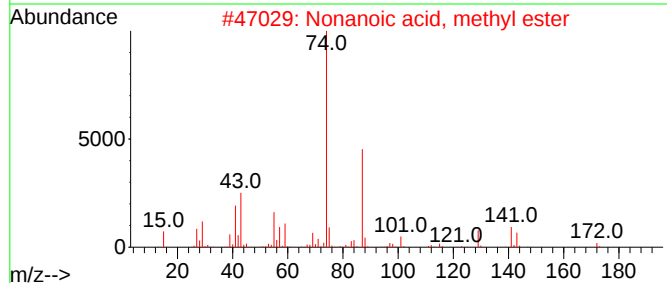
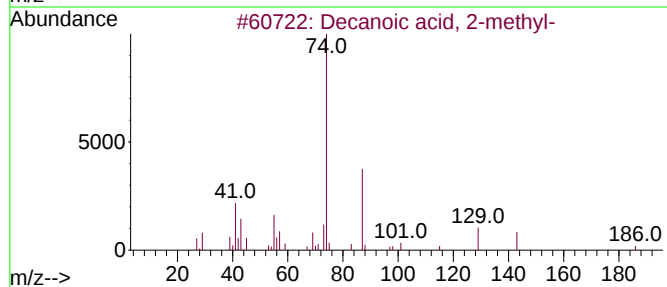
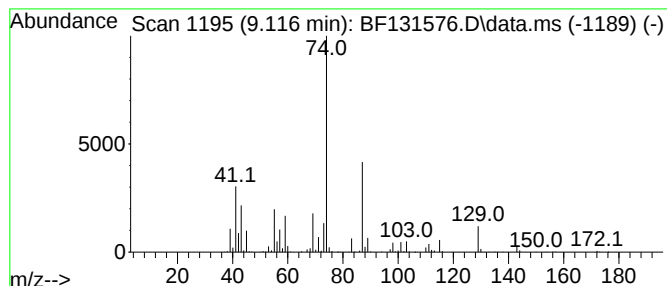
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Decanoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.116	154.40 ng	5286390	Acenaphthene-d10	9.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanoic acid, 2-methyl-	186	C11H22O2	024323-23-7	72
2			Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	64
3			Heptanoic acid, methyl ester	144	C8H16O2	000106-73-0	59
4			Methyl-2-O-methyl.alpha.d-glucop...	208	C8H16O6	015064-82-1	59
5			Undecanoic acid, 2-methyl-	200	C12H24O2	024323-25-9	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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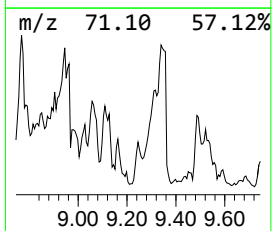
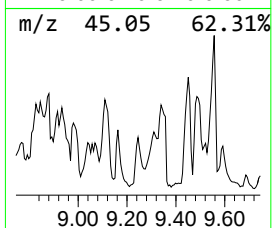
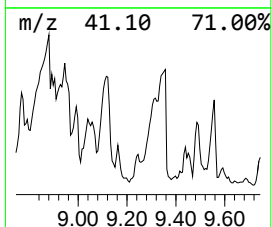
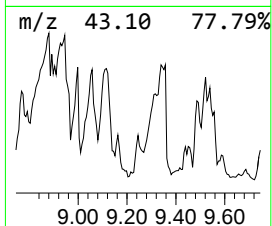
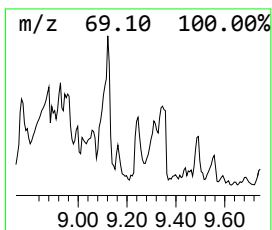
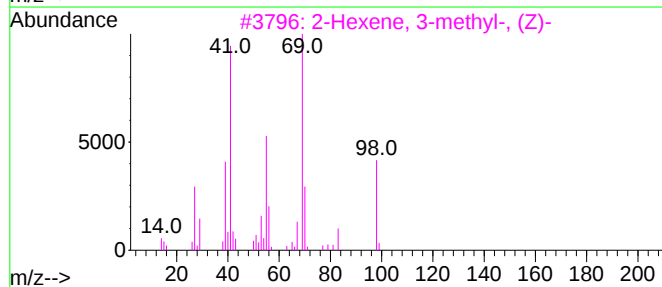
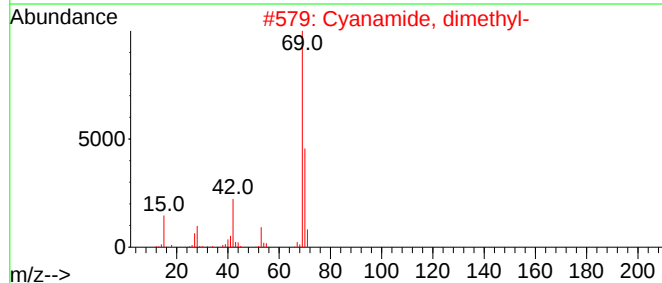
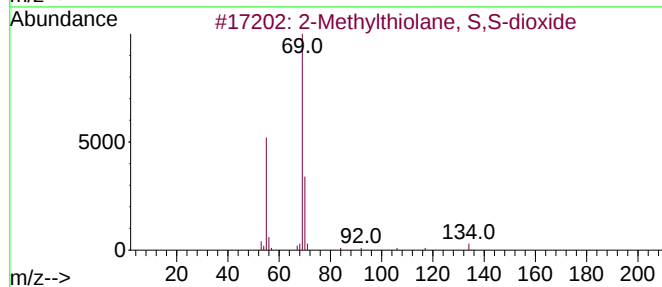
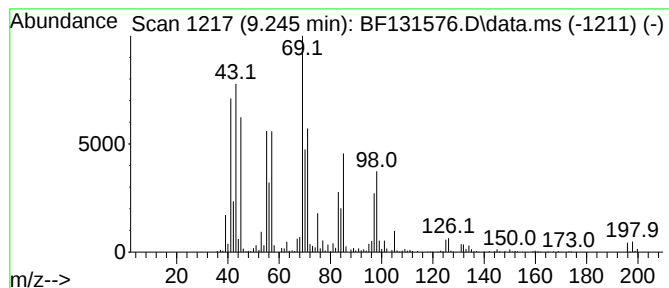
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown9.245 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.245	43.54 ng	1490680	Acenaphthene-d10	9.980

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methylthiolane, S,S-dioxide	134	C5H10O2S	001003-46-9	38
2		Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	27
3		2-Hexene, 3-methyl-, (Z)-	98	C7H14	010574-36-4	25
4		Pentadecafluorooctanoic acid, un...	568	C19H23F15O2	1010406-04-1	25
5		3-Methyl-3-hexene	98	C7H14	003404-65-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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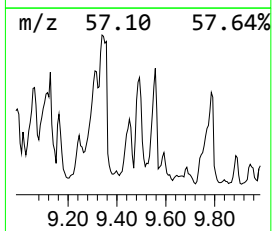
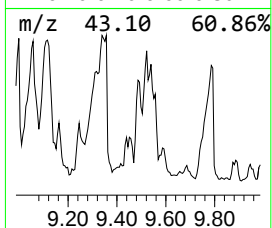
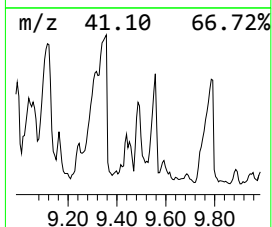
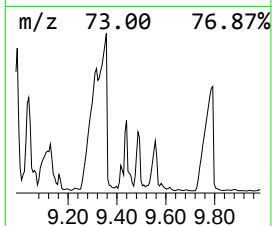
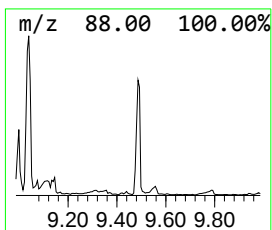
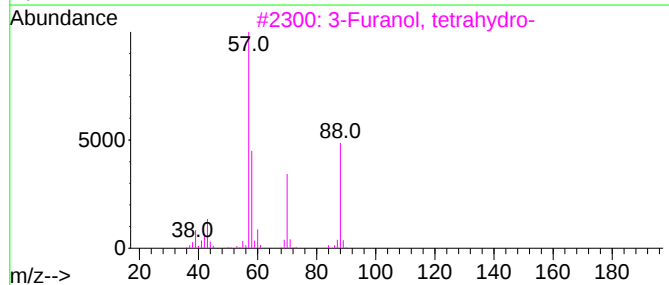
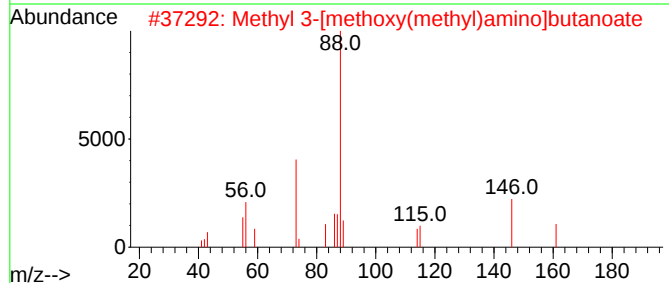
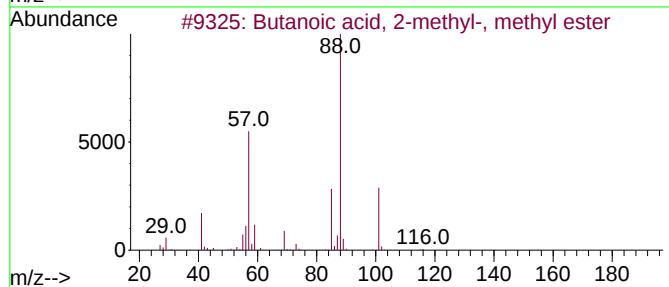
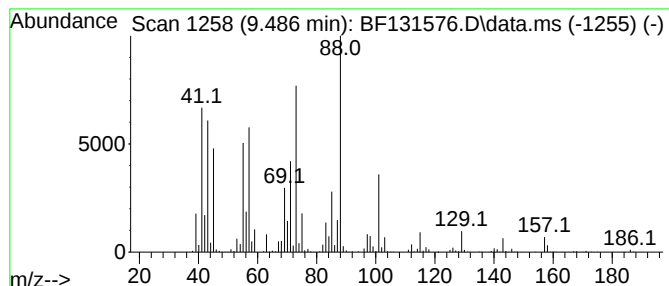
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown9.486 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.486	58.03 ng	1986920	Acenaphthene-d10	9.980

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	49
2		Methyl 3-[methoxy(methyl)amino]b...	161	C7H15NO3	959080-02-5	27
3		3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	22
4		Butanamide, N-(1-oxopropyl)-	143	C7H13NO2	032796-69-3	22
5		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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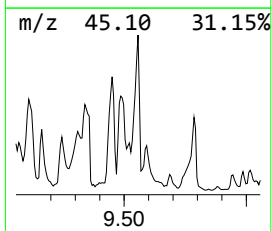
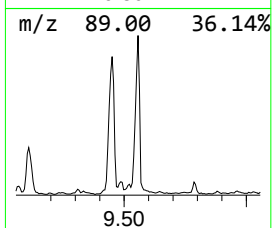
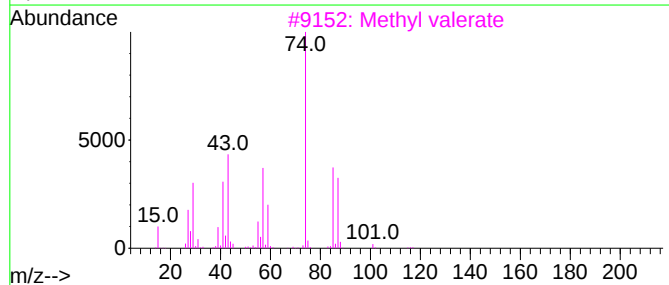
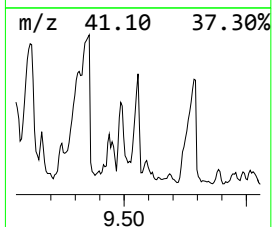
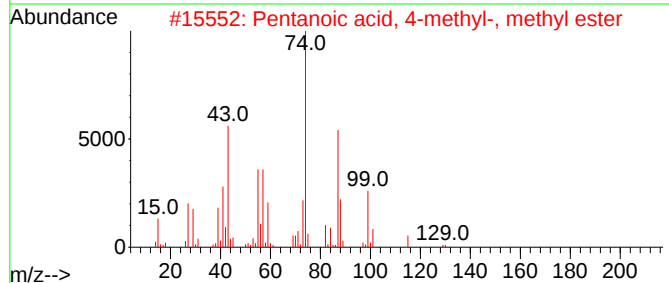
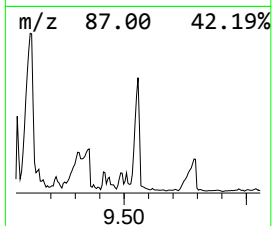
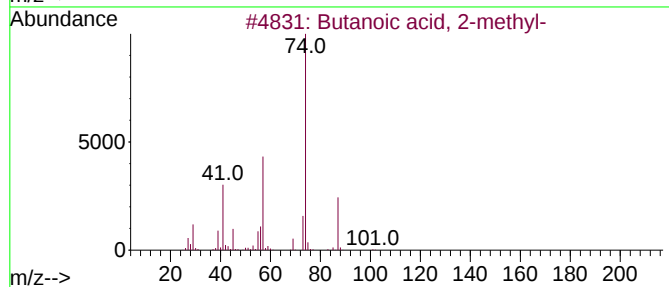
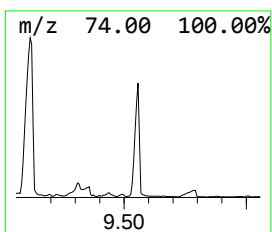
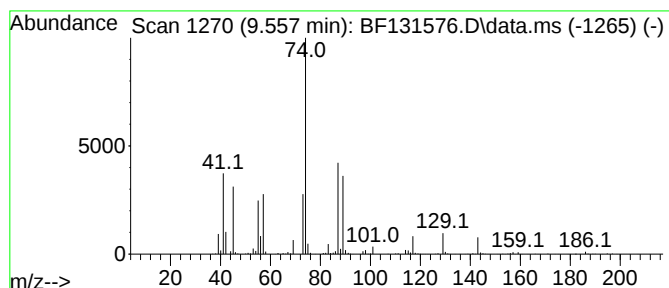
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Butanoic acid, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.557	81.80 ng	2800640	Acenaphthene-d10	9.980

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	50
2		Pentanoic acid, 4-methyl-, methy...	130	C7H14O2	002412-80-8	47
3		Methyl valerate	116	C6H12O2	000624-24-8	47
4		Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	43
5		Undecanoic acid, 2-methyl-	200	C12H24O2	024323-25-9	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
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Acq On : 09 Dec 2022 20:17
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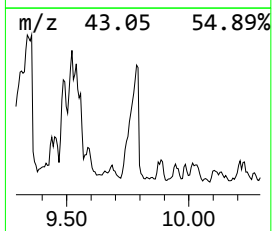
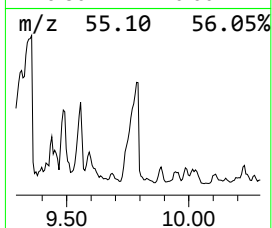
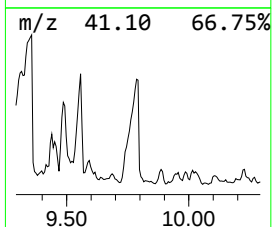
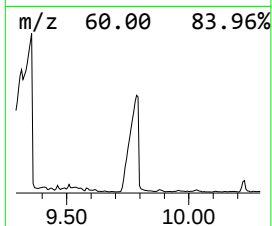
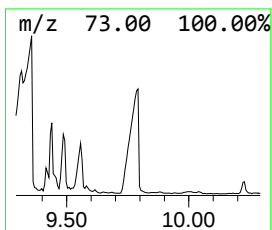
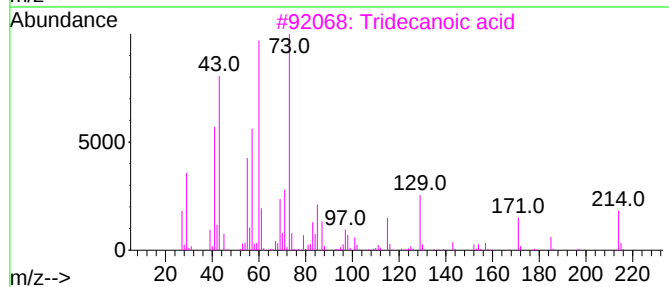
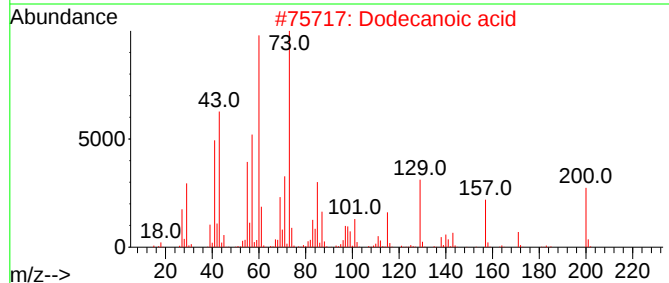
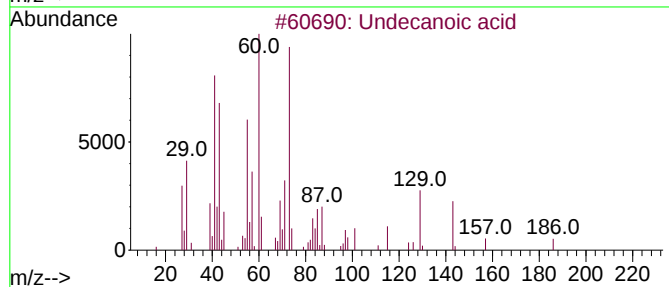
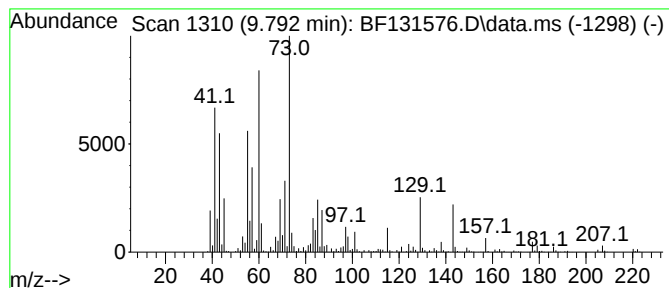
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.792	148.58 ng	5087110	Acenaphthene-d10	9.980

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Undecanoic acid	186	C11H22O2	000112-37-8	91
2		Dodecanoic acid	200	C12H24O2	000143-07-7	80
3		Tridecanoic acid	214	C13H26O2	000638-53-9	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	64
5		Octanoic acid	144	C8H16O2	000124-07-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FMC-TOTE-1207

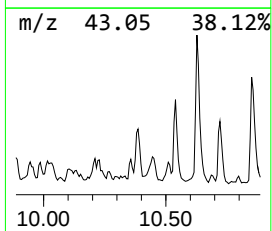
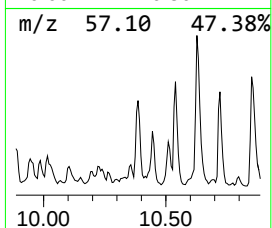
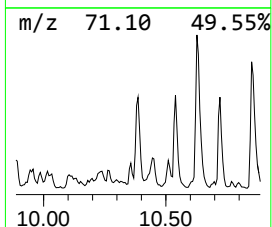
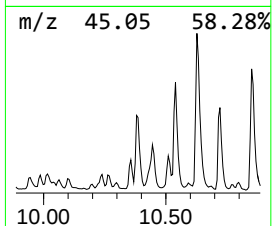
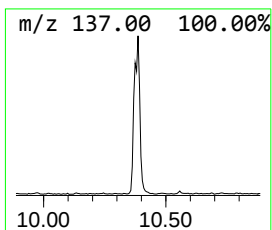
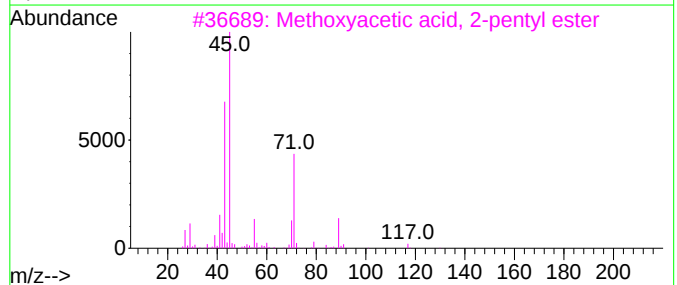
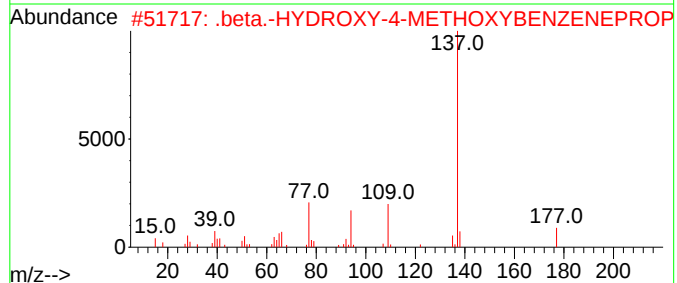
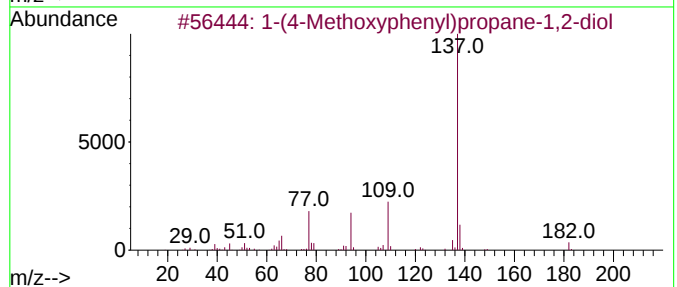
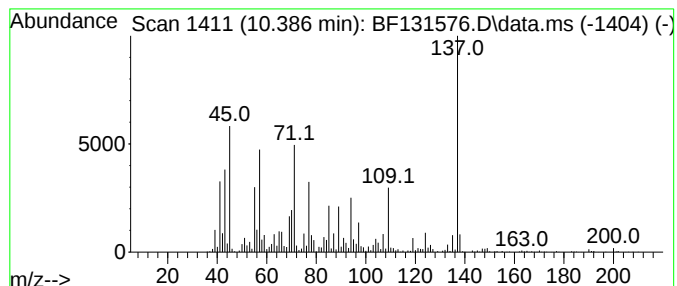
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown10.386 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.386	57.29 ng	1961660	Acenaphthene-d10	9.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(4-Methoxyphenyl)propane-1,2-diol	182	C10H14O3	051410-48-1	38
2			.beta.-HYDROXY-4-METHOXYBENZENEPROP	177	C10H11NO2	051241-27-1	35
3			Methoxyacetic acid, 2-pentyl ester	160	C8H16O3	1000282-69-2	27
4			2-Hydroxy-2-(4-methoxy-phenyl)-N...	195	C10H13NO3	087920-02-3	27
5			4-Methoxyphenylethyleneglycol	168	C9H12O3	013603-63-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FMC-TOTE-1207

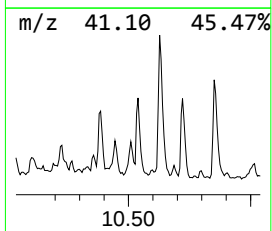
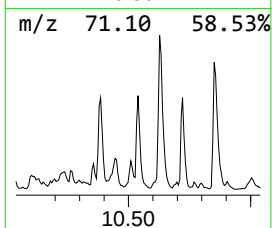
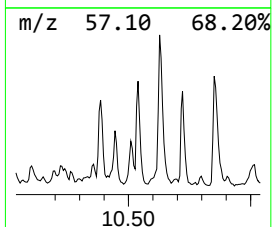
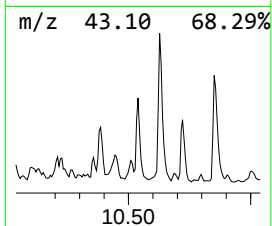
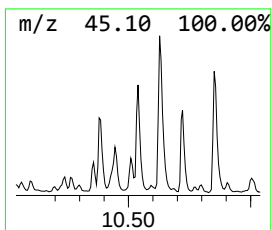
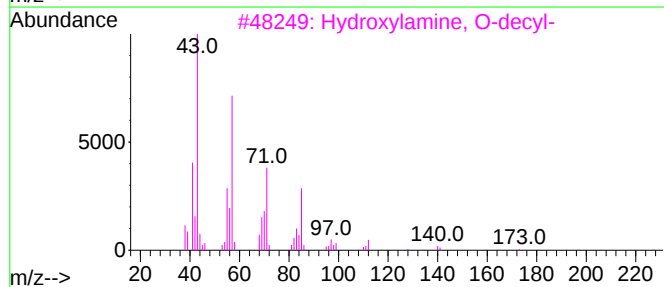
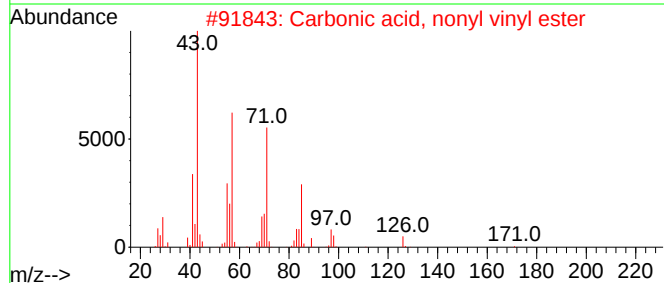
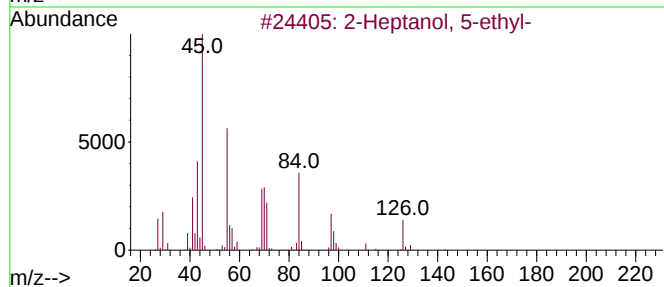
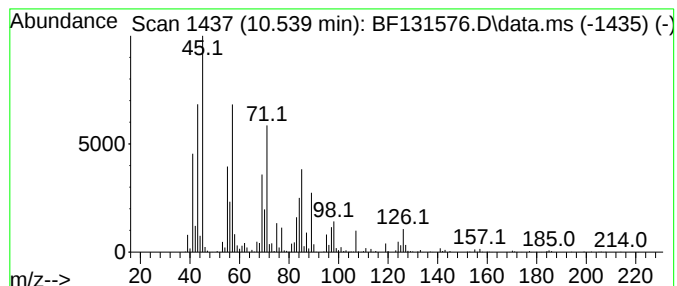
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown10.539 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.539	31.15 ng	1066380	Acenaphthene-d10	9.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanol, 5-ethyl-		144	C9H20O	019780-40-6	47	
2	Carbonic acid, nonyl vinyl ester		214	C12H22O3	1000383-25-6	43	
3	Hydroxylamine, O-decyl-		173	C10H23NO	029812-79-1	35	
4	Carbonic acid, prop-1-en-2-yl te...		298	C18H34O3	1000382-90-9	35	
5	Propanoic acid, 2-methyl-, penty...		158	C9H18O2	002445-72-9	35	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

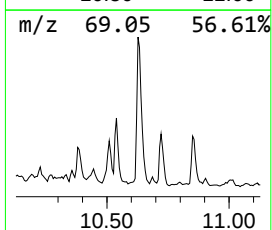
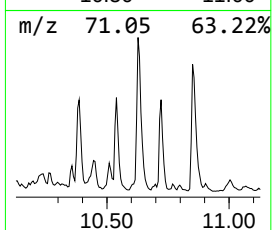
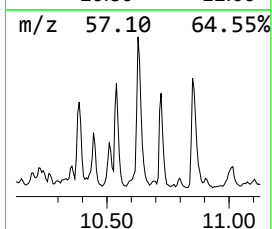
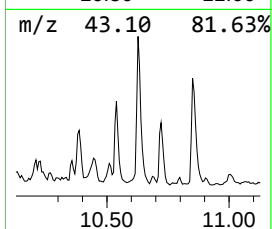
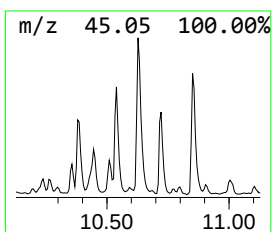
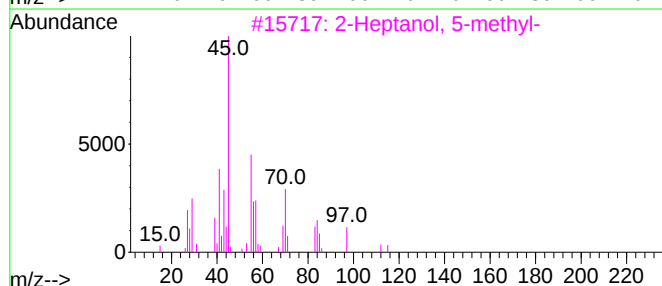
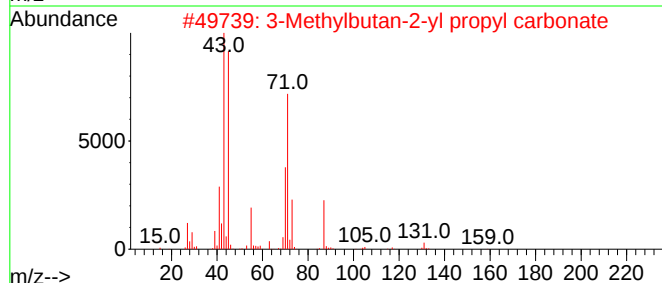
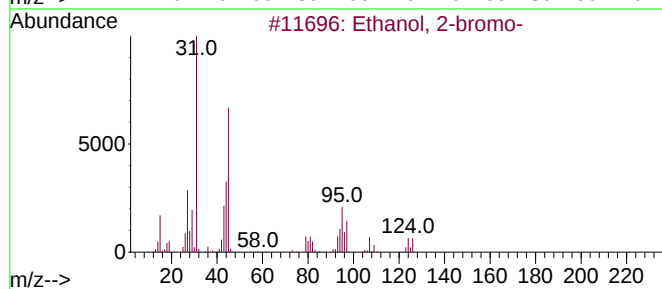
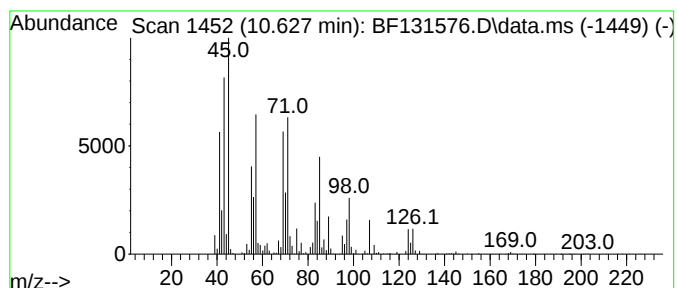
Instrument :
BNA_F
ClientSampleId :
FMC-TOTE-1207

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown10.627 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.627	65.36 ng	2237790	Acenaphthene-d10	9.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-bromo-	124	C2H5BrO	000540-51-2	38
2	3-Methylbutan-2-yl propyl carbonate	174	C9H18O3	1000372-83-4	38
3	2-Heptanol, 5-methyl-	130	C8H18O	054630-50-1	35
4	Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	27
5	Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131576.D
Acq On : 09 Dec 2022 20:17
Operator : CG\JU
Sample : N5912-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FMC-TOTE-1207

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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...	2.193	43.8	ng	1652280	1	6.916	755202	20.0
Ethanol, 2-butoxy-	5.922	181.2	ng	6842010	1	6.916	755202	20.0
Pentanoic acid	6.069	28.9	ng	1093320	1	6.916	755202	20.0
2-Propanol, 1-b...	6.286	284.7	ng	10750800	1	6.916	755202	20.0
Butane, 1-(1-me...	6.410	61.2	ng	2311640	1	6.916	755202	20.0
Eucalyptol	7.075	43.8	ng	1653430	1	6.916	755202	20.0
Hexanoic acid, ...	8.392	181.3	ng	23242200	2	8.204	2564240	20.0
2-Propanol, 1-[...	8.504	419.8	ng	53816600	2	8.204	2564240	20.0
1-Propanol, 2-(...	8.716	29.4	ng	3775380	2	8.204	2564240	20.0
unknown8.857	8.857	37.0	ng	4747600	2	8.204	2564240	20.0
Indole	8.933	30.7	ng	3933770	2	8.204	2564240	20.0
Decanoic acid, ...	9.116	154.4	ng	5286390	3	9.980	684775	20.0
unknown9.245	9.245	43.5	ng	1490680	3	9.980	684775	20.0
unknown9.486	9.486	58.0	ng	1986920	3	9.980	684775	20.0
Butanoic acid, ...	9.557	81.8	ng	2800640	3	9.980	684775	20.0
Undecanoic acid	9.792	148.6	ng	5087110	3	9.980	684775	20.0
unknown10.386	10.386	57.3	ng	1961660	3	9.980	684775	20.0
unknown10.539	10.539	31.1	ng	1066380	3	9.980	684775	20.0
unknown10.627	10.627	65.4	ng	2237790	3	9.980	684775	20.0
n-Octylpentaoxy...	14.904	42.1	ng	3572580	6	15.633	1695340	20.0