

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
 Data File : BF131474.D
 Acq On : 30 Nov 2022 16:41
 Operator : CG\JU
 Sample : N5799-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 220-1-STONES

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-BF112122.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131474.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	21	28	34	rVB	520264	670326	25.85%	2.871%
2	2.363	40	47	49	rBV	44206	63208	2.44%	0.271%
3	2.387	49	51	56	rVB	41858	46467	1.79%	0.199%
4	4.551	415	419	423	rBV	75332	79698	3.07%	0.341%
5	5.175	512	525	528	rBV	1360340	1730651	66.75%	7.412%
6	5.563	586	591	594	rBV	2059174	1975518	76.19%	8.461%
7	5.628	594	602	607	rVB2	28580	70215	2.71%	0.301%
8	5.740	618	621	623	rBV	53220	43704	1.69%	0.187%
9	5.957	655	658	663	rVB	157557	126085	4.86%	0.540%
10	6.110	681	684	687	rBV	49109	45988	1.77%	0.197%
11	6.375	724	729	732	rVB2	69424	66685	2.57%	0.286%
12	6.569	747	762	765	rBV	1799613	2012600	77.62%	8.619%
13	6.657	775	777	781	rVB	116130	81520	3.14%	0.349%
14	6.945	822	826	829	rBV	691630	571781	22.05%	2.449%
15	7.140	852	859	860	rBV	48034	95389	3.68%	0.409%
16	7.157	860	862	867	rVB	152139	118582	4.57%	0.508%
17	7.304	880	887	890	rVV2	64301	85785	3.31%	0.367%
18	7.345	891	894	898	rVB3	34353	41578	1.60%	0.178%
19	7.510	917	922	925	rVB	1436387	1403503	54.13%	6.011%
20	7.792	965	970	972	rBV4	47007	64095	2.47%	0.274%
21	7.828	972	976	978	rVB	81920	88915	3.43%	0.381%
22	7.975	989	1001	1004	rBV3	136803	247429	9.54%	1.060%
23	8.051	1010	1014	1015	rBV4	38676	46149	1.78%	0.198%
24	8.139	1026	1029	1035	rBV3	174262	247208	9.53%	1.059%
25	8.234	1041	1045	1048	rBV	913618	817511	31.53%	3.501%
26	8.269	1048	1051	1055	rVV3	33799	51018	1.97%	0.218%
27	8.345	1060	1064	1066	rVV	88223	98809	3.81%	0.423%
28	8.422	1070	1077	1082	rVB5	48273	84912	3.27%	0.364%
29	8.504	1088	1091	1093	rBV2	32818	42051	1.62%	0.180%
30	8.539	1093	1097	1100	rVV2	65724	90790	3.50%	0.389%
31	8.592	1100	1106	1108	rVV	246199	309831	11.95%	1.327%
32	8.651	1111	1116	1122	rVB5	96684	145188	5.60%	0.622%
33	8.757	1131	1134	1137	rVB2	45973	51782	2.00%	0.222%
34	8.786	1137	1139	1141	rBV	39256	43007	1.66%	0.184%
35	8.857	1149	1151	1154	rVB3	42935	42390	1.63%	0.182%
36	8.916	1157	1161	1162	rBV4	52324	60753	2.34%	0.260%

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37	8.934	1162	1164	1166	rVB2	61060	45990	1.77%	0.197%
38	9.004	1172	1176	1180	rBV2	59438	76273	2.94%	0.327%
39	9.075	1184	1188	1191	rBV4	55255	83805	3.23%	0.359%
40	9.157	1199	1202	1205	rBV	213033	233271	9.00%	0.999%
41	9.222	1208	1213	1216	rBV5	51899	72644	2.80%	0.311%
42	9.251	1216	1218	1222	rVB4	71663	70346	2.71%	0.301%
43	9.316	1224	1229	1232	rBV	2817993	2592830	100.00%	11.104%
44	9.386	1236	1241	1243	rBV5	71832	90312	3.48%	0.387%
45	9.410	1243	1245	1248	rVB2	86776	70565	2.72%	0.302%
46	9.486	1255	1258	1262	rVB3	75699	80187	3.09%	0.343%
47	9.681	1287	1291	1292	rBV	146667	168528	6.50%	0.722%
48	9.698	1292	1294	1300	rVB3	232392	289788	11.18%	1.241%
49	9.757	1302	1304	1308	rVB4	50440	41472	1.60%	0.178%
50	9.810	1311	1313	1316	rBV2	58884	64340	2.48%	0.276%
51	9.904	1327	1329	1334	rVB3	98187	119609	4.61%	0.512%
52	9.945	1334	1336	1339	rBV3	53592	71624	2.76%	0.307%
53	10.004	1342	1346	1349	rBV	976339	858166	33.10%	3.675%
54	10.069	1354	1357	1364	rBV7	47373	97512	3.76%	0.418%
55	10.128	1364	1367	1370	rBV3	50580	85264	3.29%	0.365%
56	10.180	1374	1376	1378	rVV3	99954	88509	3.41%	0.379%
57	10.210	1378	1381	1385	rVB2	225209	194445	7.50%	0.833%
58	10.251	1385	1388	1391	rBV2	154882	170469	6.57%	0.730%
59	10.280	1391	1393	1397	rVB2	80655	82418	3.18%	0.353%
60	10.410	1412	1415	1416	rBV2	107483	99322	3.83%	0.425%
61	10.651	1453	1456	1460	rVB	189944	209896	8.10%	0.899%
62	10.798	1478	1481	1484	rBV	1432530	1275036	49.18%	5.461%
63	10.916	1497	1501	1504	rBV	752250	862783	33.28%	3.695%
64	11.392	1579	1582	1588	rVB	563568	687581	26.52%	2.945%
65	11.504	1598	1601	1604	rBV	899620	914660	35.28%	3.917%
66	13.110	1871	1874	1877	rVB	1251428	1136596	43.84%	4.868%
67	15.704	2312	2315	2322	rVB	389168	554419	21.38%	2.374%

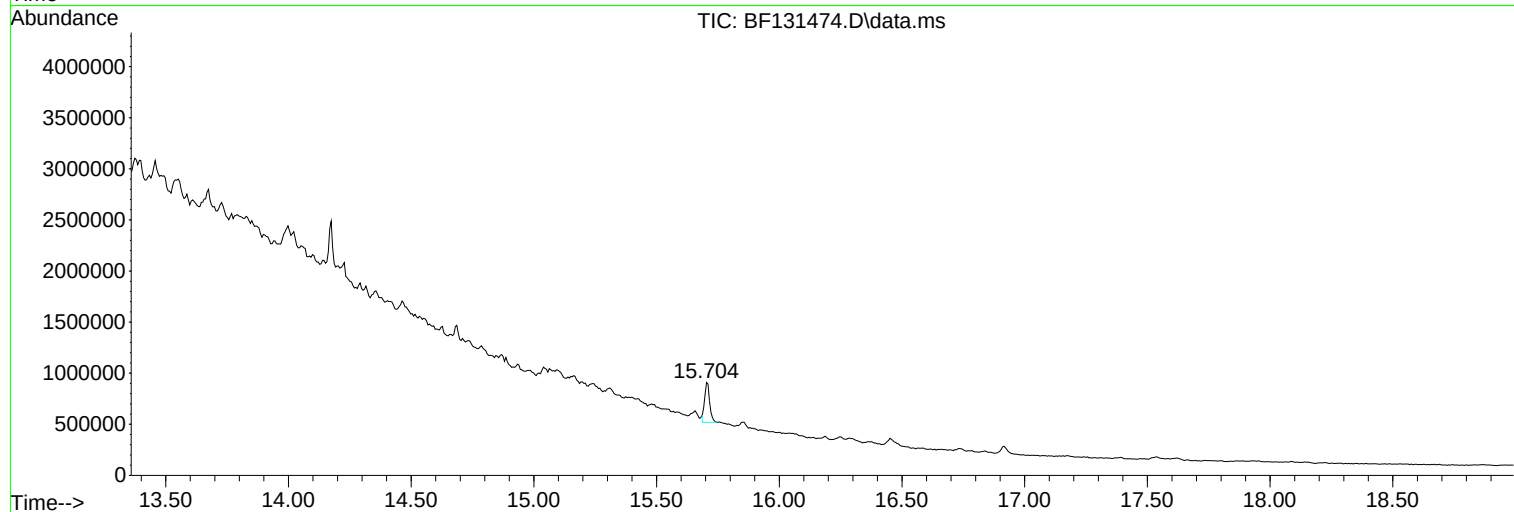
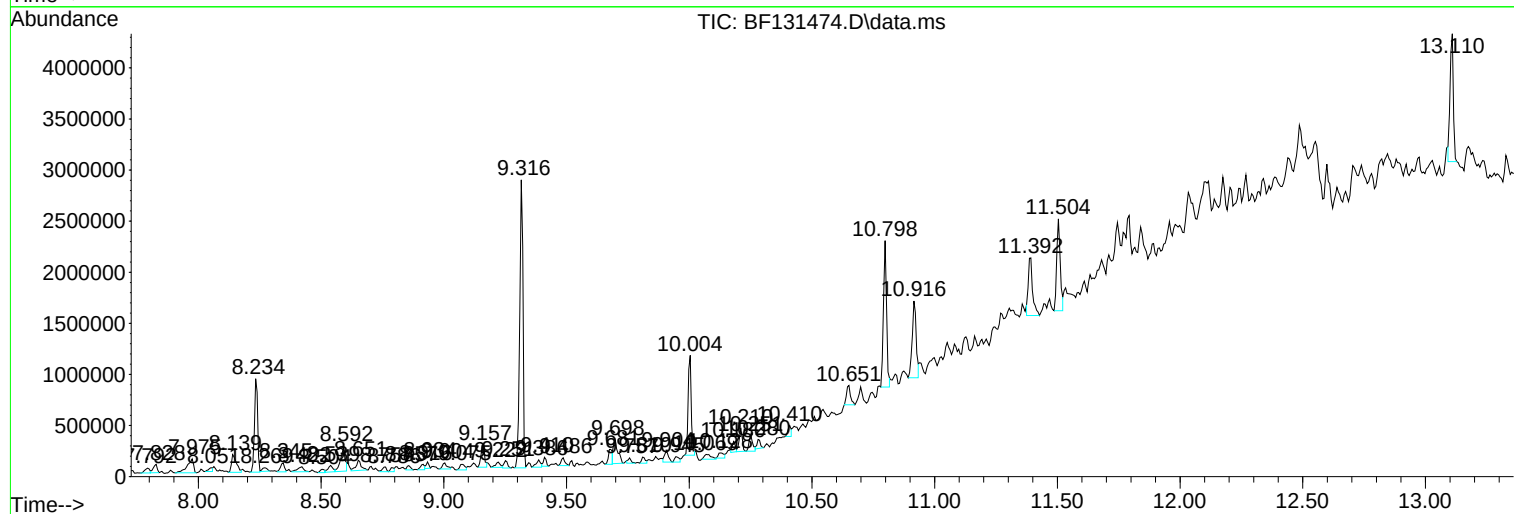
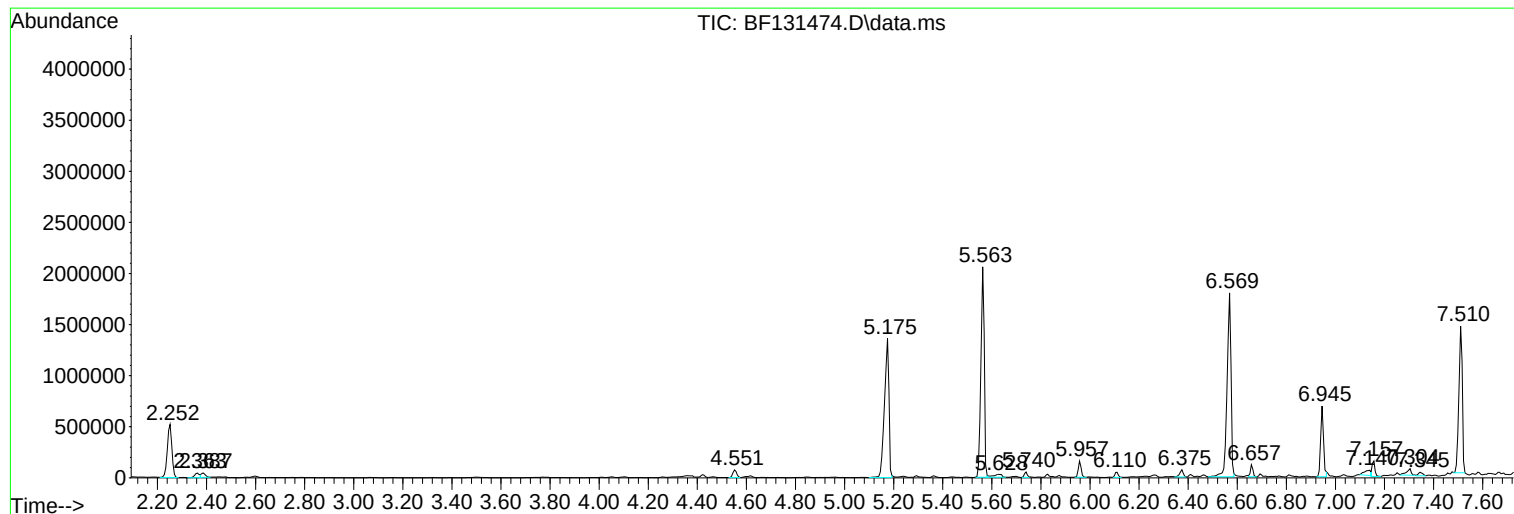
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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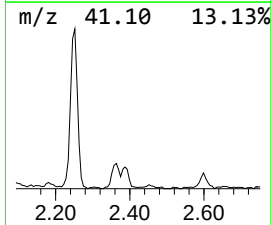
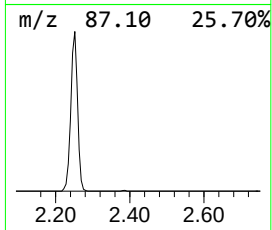
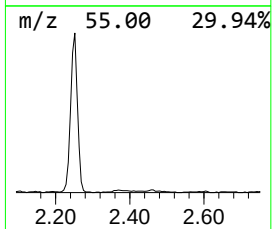
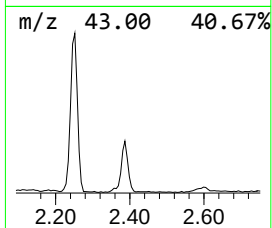
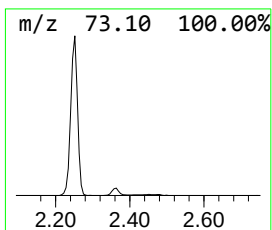
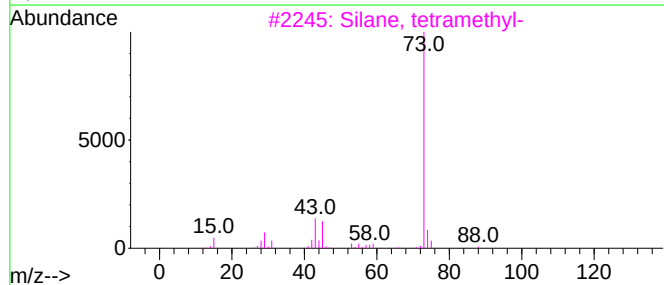
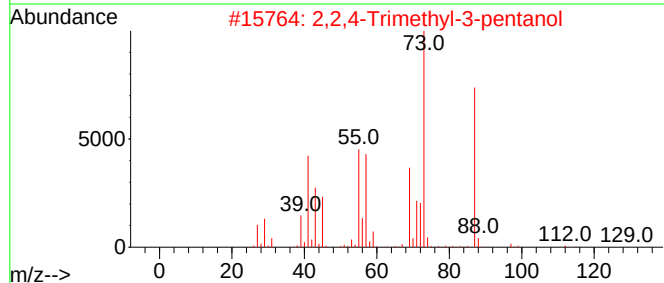
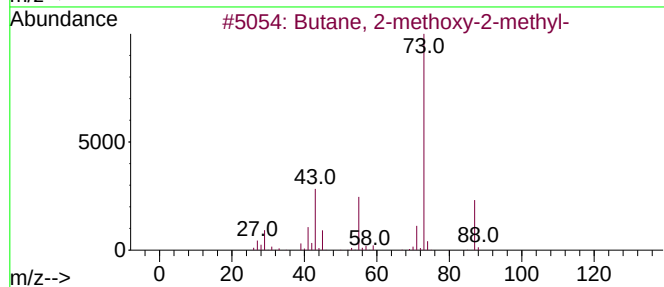
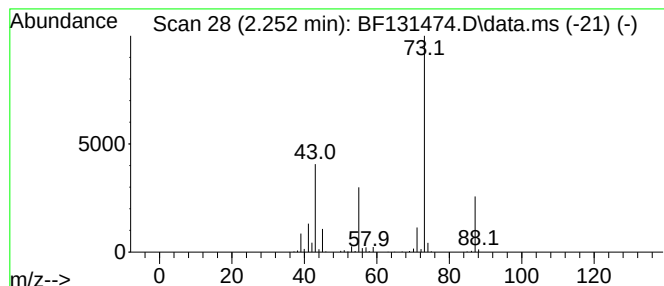
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	23.45 ng	670326	1,4-Dichlorobenzene-d4	6.945

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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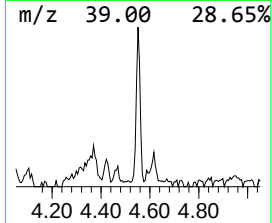
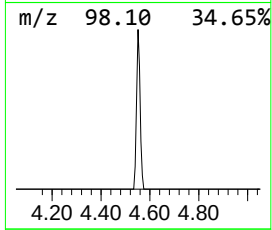
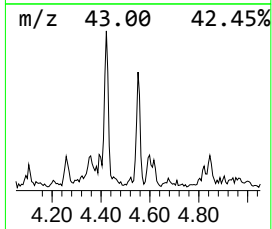
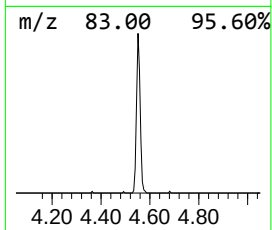
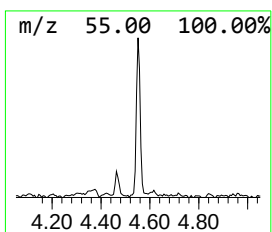
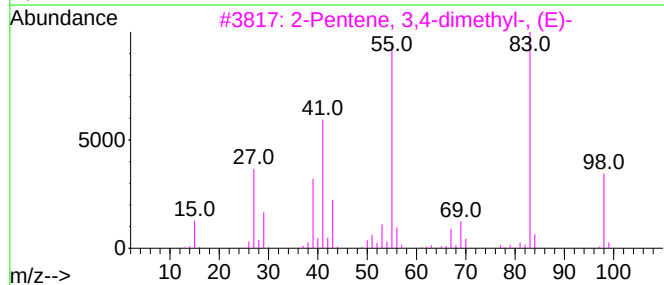
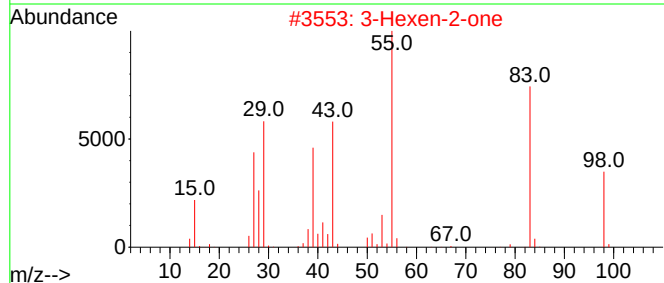
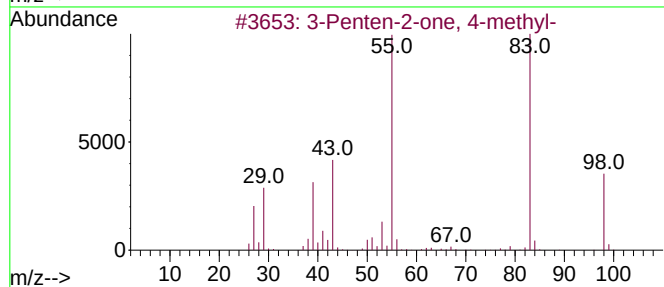
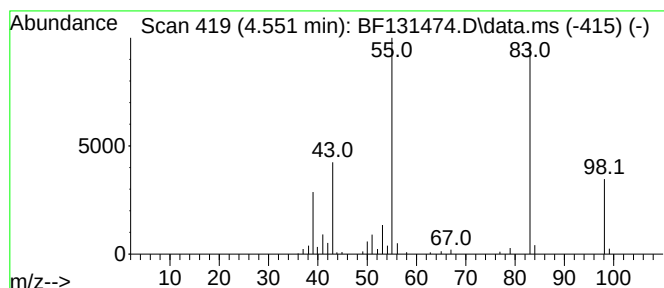
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.551	2.79 ng	79698	1,4-Dichlorobenzene-d4	6.945

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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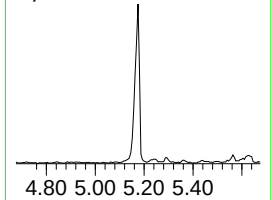
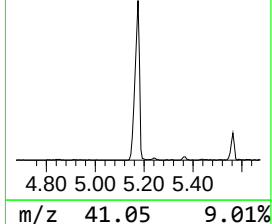
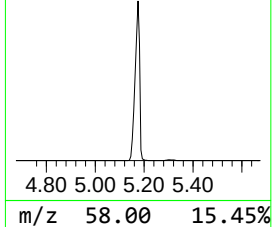
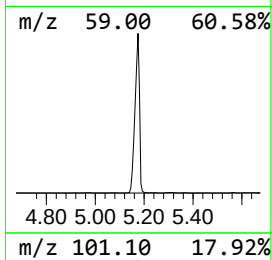
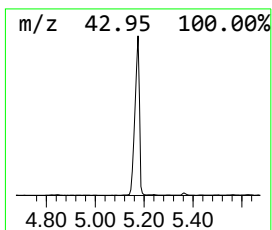
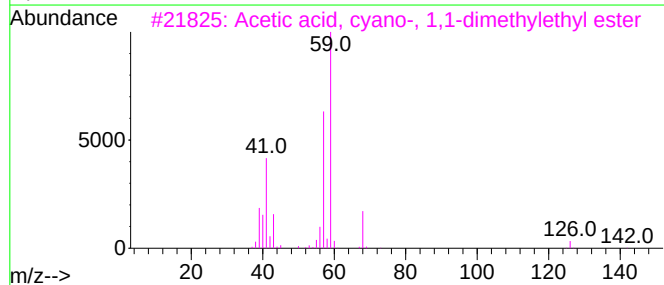
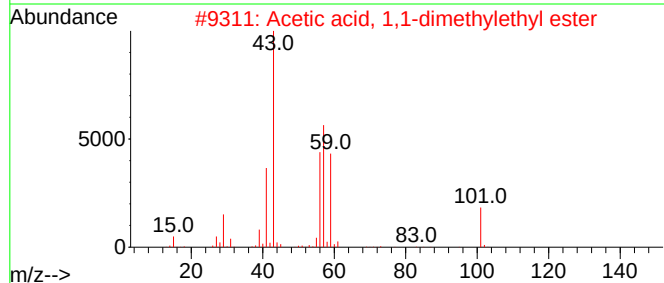
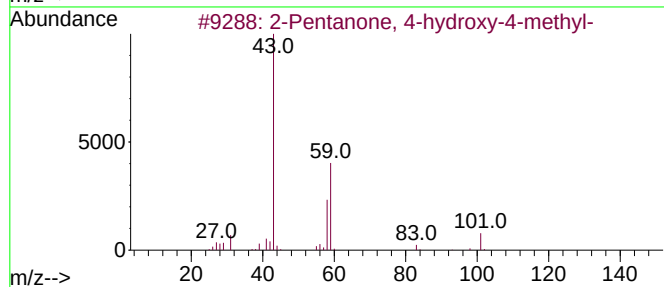
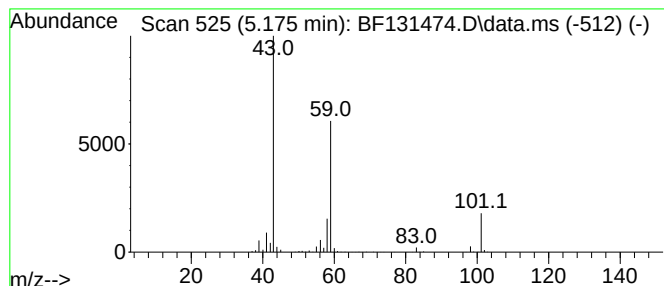
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	60.54 ng	1730650	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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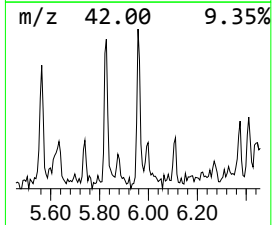
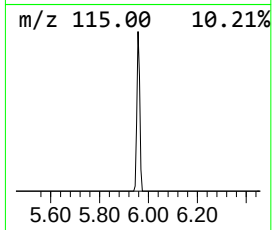
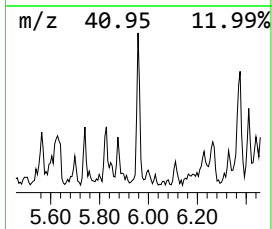
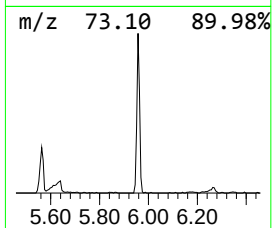
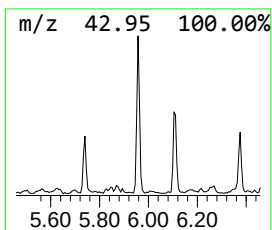
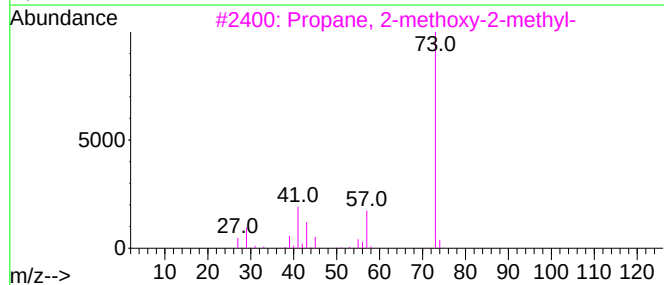
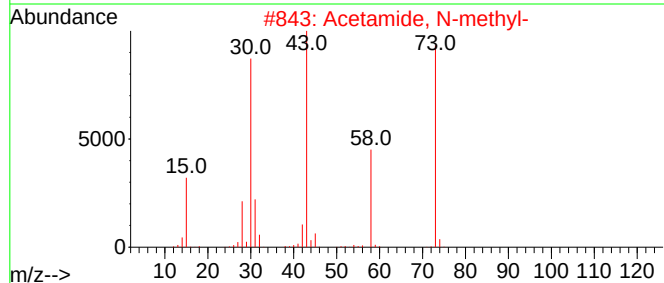
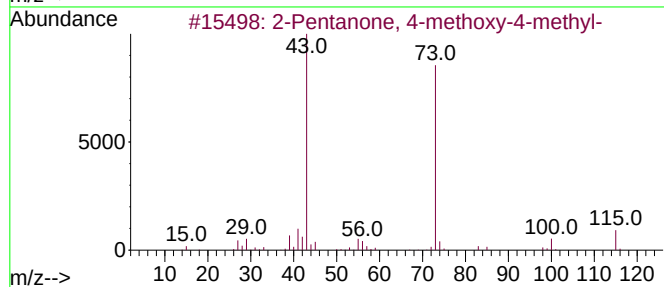
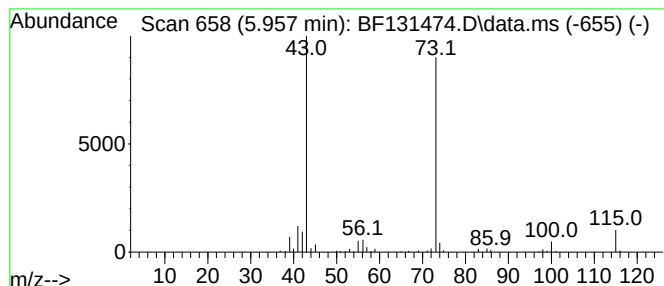
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.957	4.41 ng	126085	1,4-Dichlorobenzene-d4	6.945

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	38
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
4		N-Formylmorpholine	115	C5H9NO2	004394-85-8	12
5		3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131474.D
Acq On : 30 Nov 2022 16:41
Operator : CG\JU
Sample : N5799-01
Misc :
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Instrument :
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ClientSampleId :
220-1-STONES

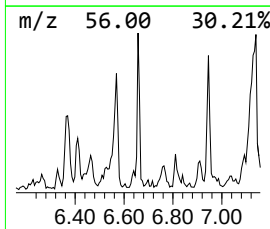
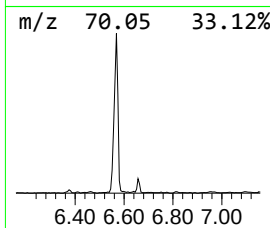
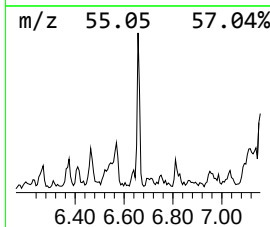
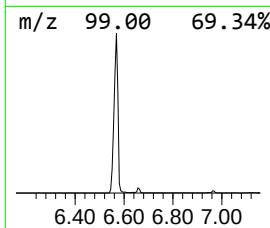
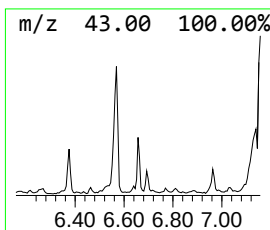
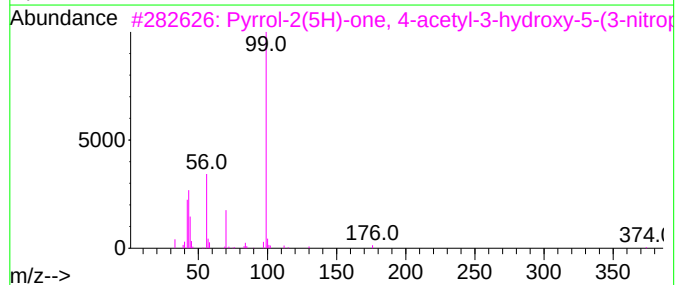
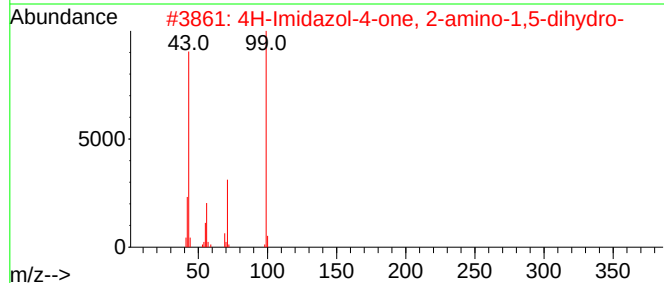
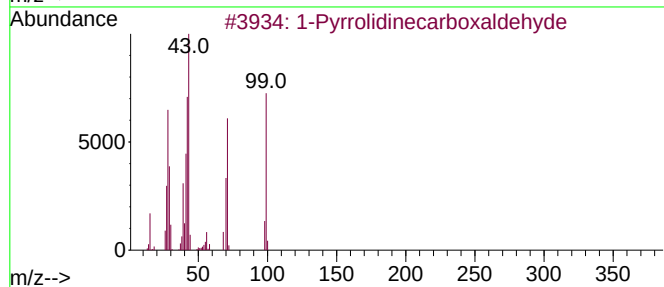
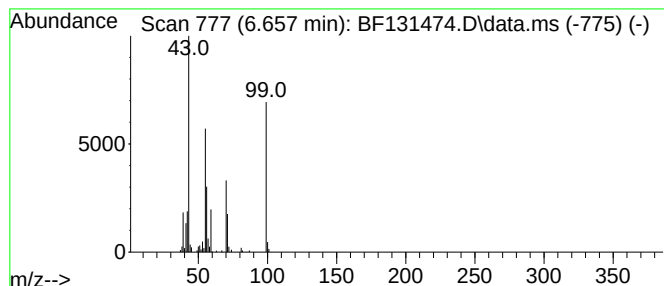
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.657 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.657	2.85 ng	81520	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	47
2			4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	43
3			Pyrrol-2(5H)-one, 4-acetyl-3-hyd...	374	C18H22N4O5	302566-41-2	37
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	35
5			1H-1,2,3,4-Tetrazol-5-amine, 1-m...	99	C2H5N5	005422-44-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131474.D
Acq On : 30 Nov 2022 16:41
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ClientSampleId :
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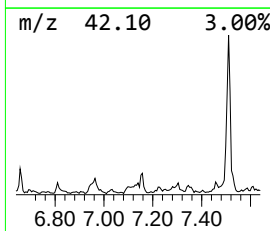
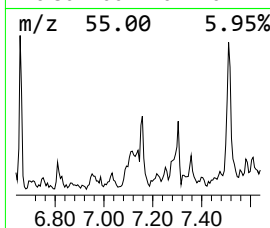
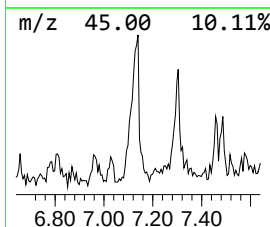
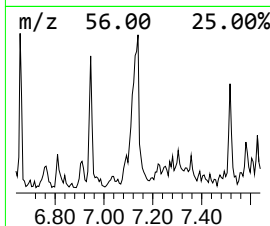
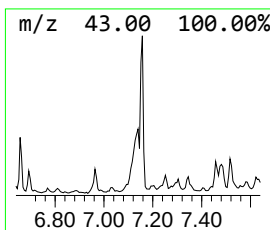
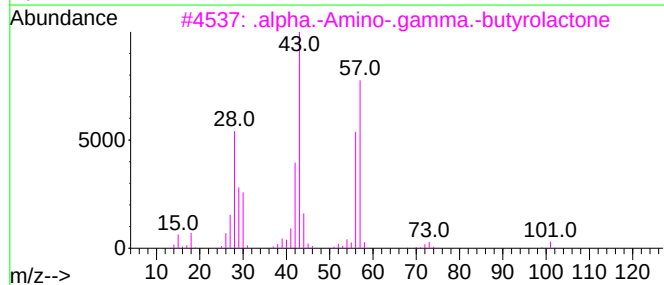
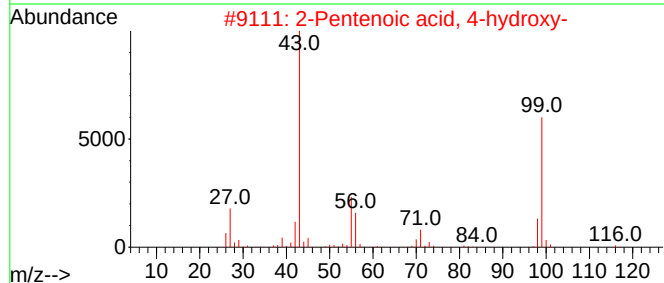
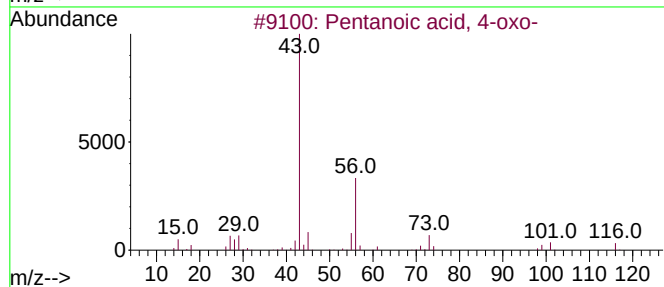
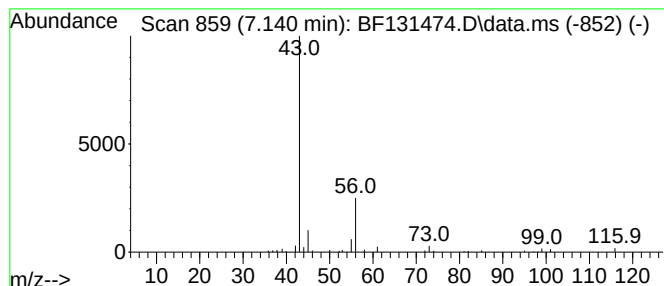
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown7.140 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.140	3.34 ng	95389	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	36
2			2-Pentenoic acid, 4-hydroxy-	116	C5H8O3	028525-83-9	9
3			.alpha.-Amino-.gamma.-butyrolactone	101	C4H7NO2	001192-20-7	7
4			2-Propanone, 1-(acetyloxy)-	116	C5H8O3	000592-20-1	5
5			Methyl glyoxal	72	C3H4O2	000078-98-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131474.D
Acq On : 30 Nov 2022 16:41
Operator : CG\JU
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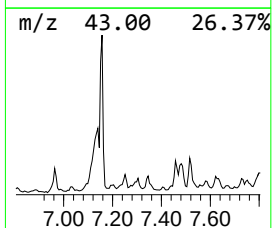
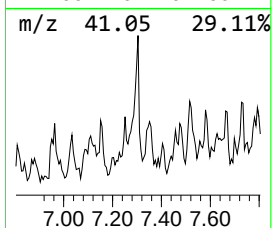
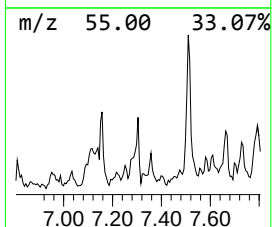
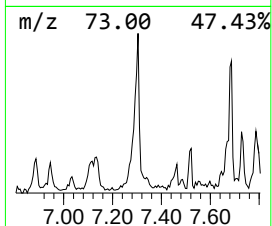
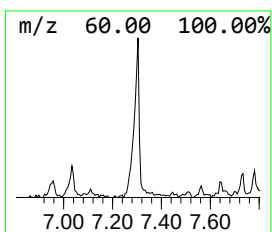
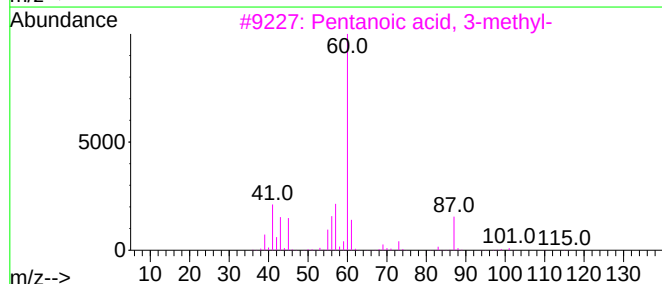
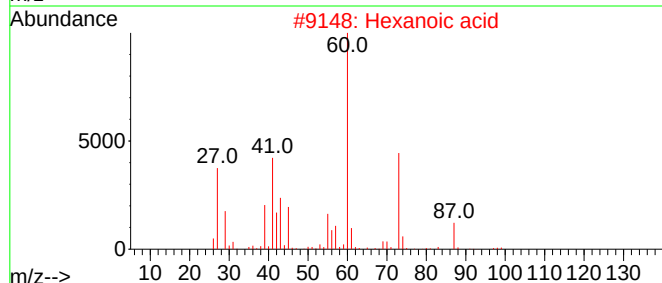
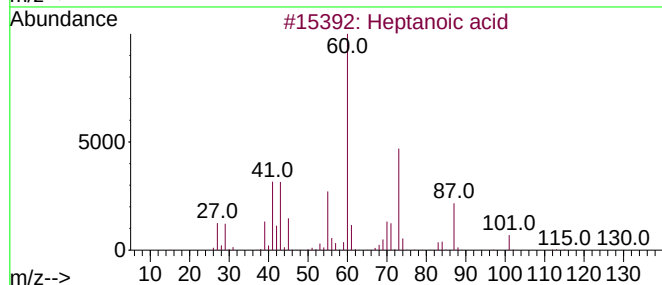
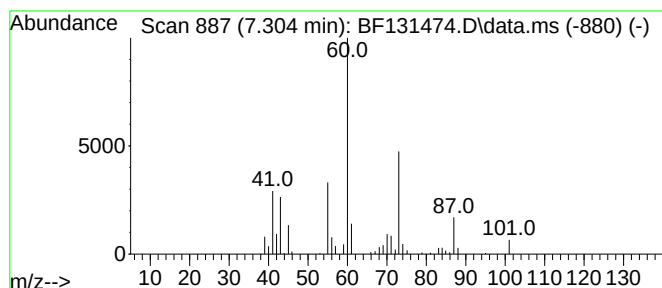
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.304	3.00 ng	85785	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanoic acid	130	C7H14O2	000111-14-8	90
2			Hexanoic acid	116	C6H12O2	000142-62-1	78
3			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	72
4			Pentanoic acid	102	C5H10O2	000109-52-4	64
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131474.D
Acq On : 30 Nov 2022 16:41
Operator : CG\JU
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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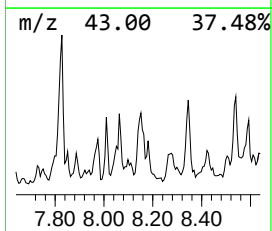
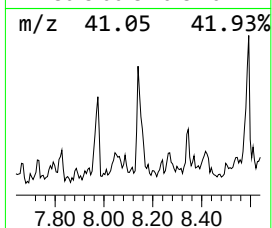
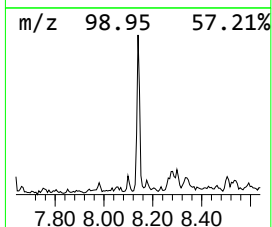
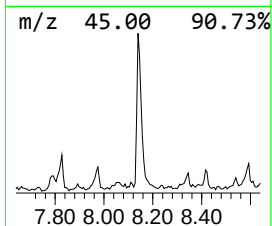
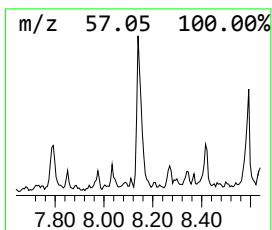
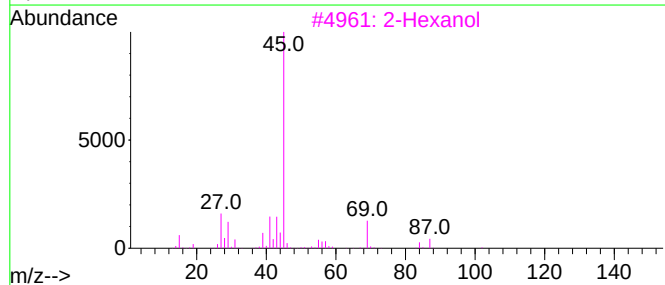
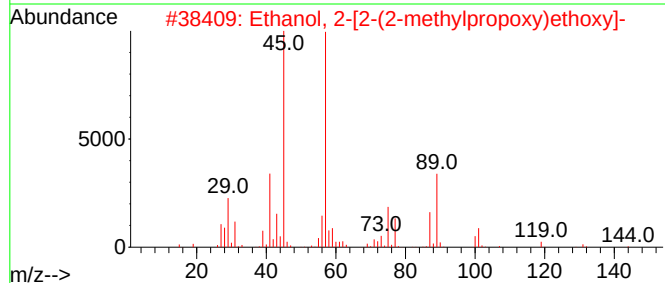
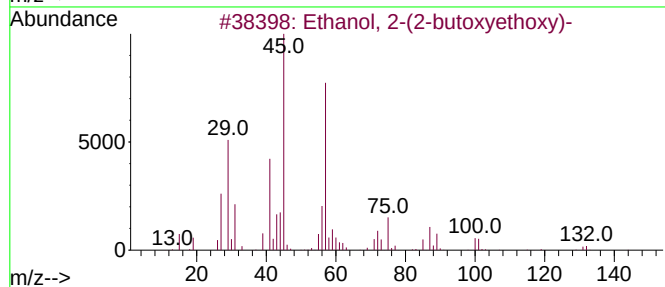
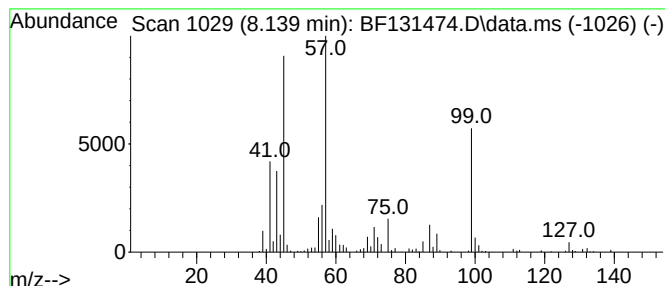
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.139	6.05 ng	247208	Naphthalene-d8	8.234

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	59
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	53
3			2-Hexanol	102	C6H14O	000626-93-7	43
4			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	43
5			2-Propanol, 1-(2-butoxyethoxy)-	176	C9H20O3	000124-16-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
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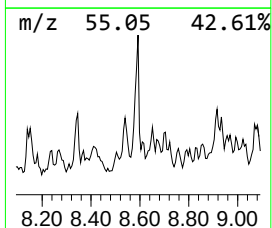
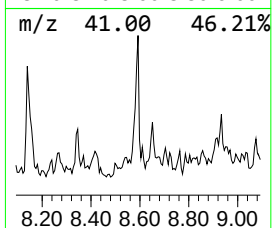
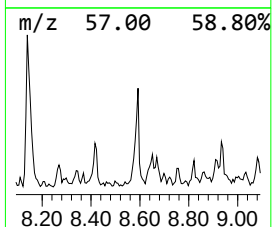
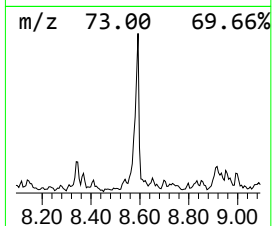
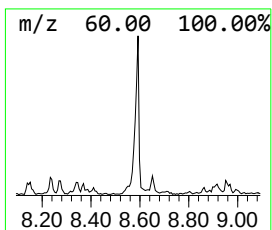
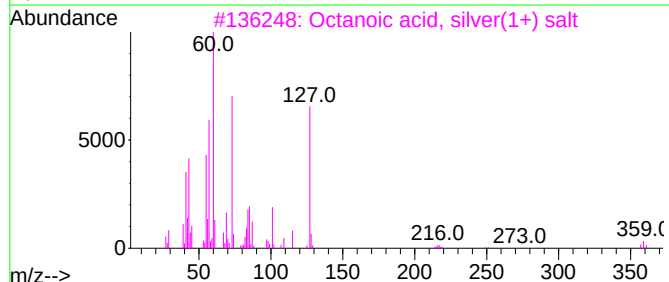
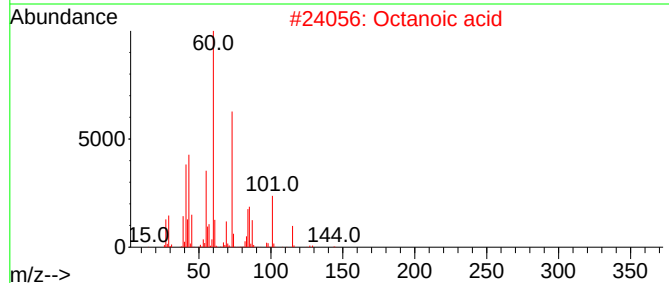
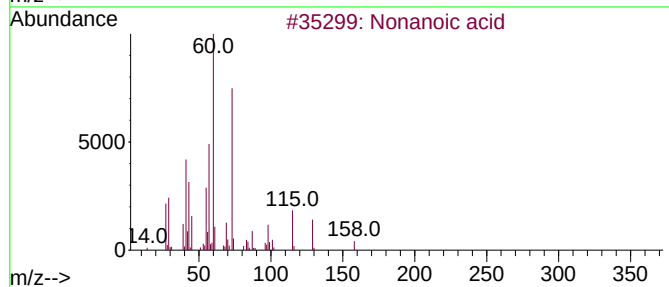
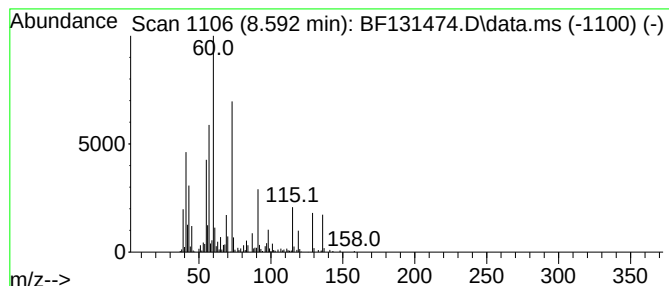
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.592	7.58 ng	309831	Naphthalene-d8	8.234

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonanoic acid	158	C9H18O2	000112-05-0	56
2		Octanoic acid	144	C8H16O2	000124-07-2	47
3		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47
4		Pentanoic acid	102	C5H10O2	000109-52-4	43
5		Hexanoic acid	116	C6H12O2	000142-62-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
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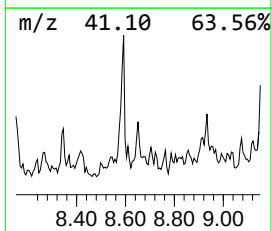
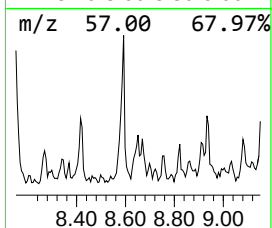
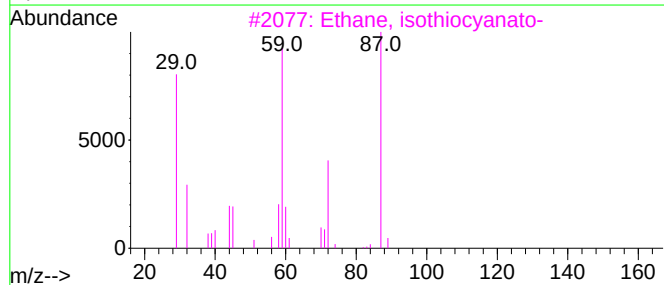
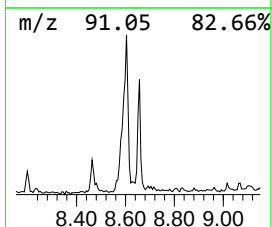
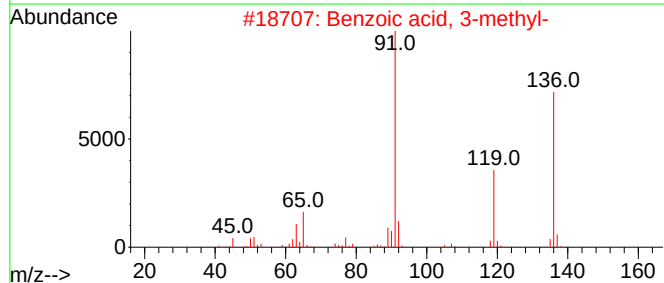
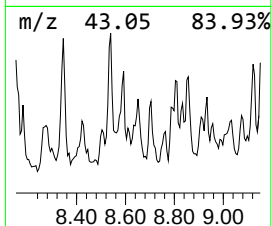
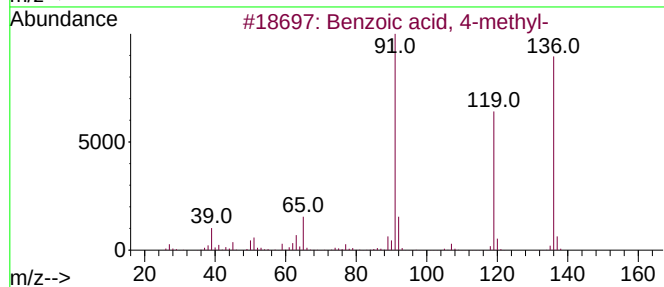
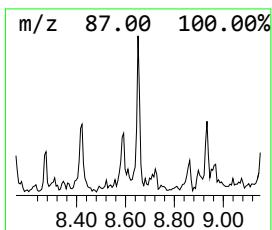
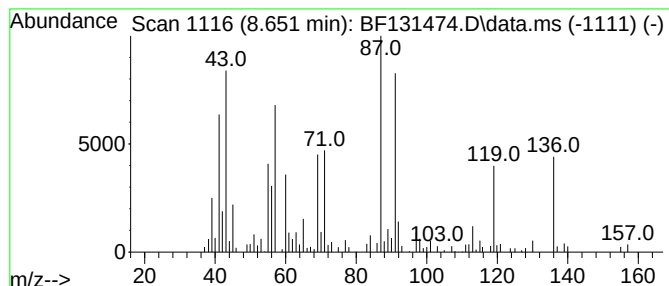
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown8.651 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.651	3.55 ng	145188	Naphthalene-d8	8.234

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	42
2			Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	22
3			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	22
4			2,2-Dimethyl-5-hexen-3-ol	128	C8H16O	019550-89-1	22
5			Pivaloin	172	C10H20O2	000815-66-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
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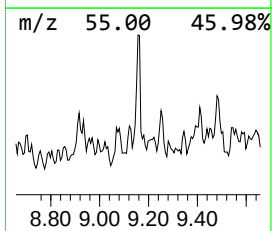
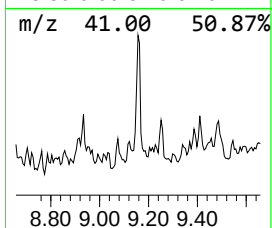
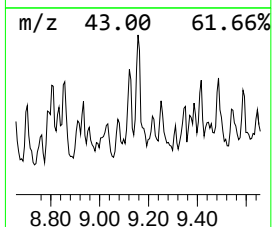
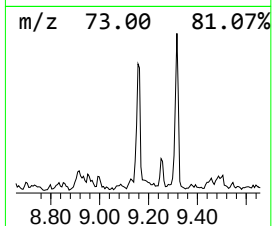
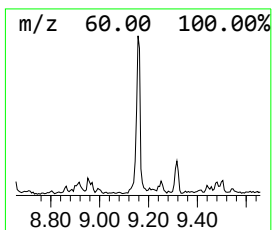
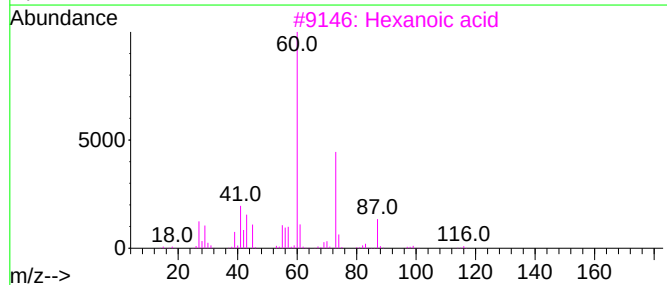
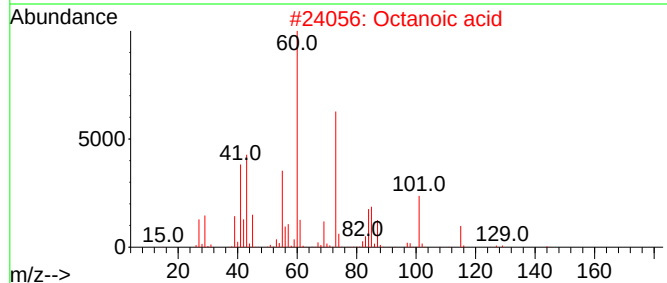
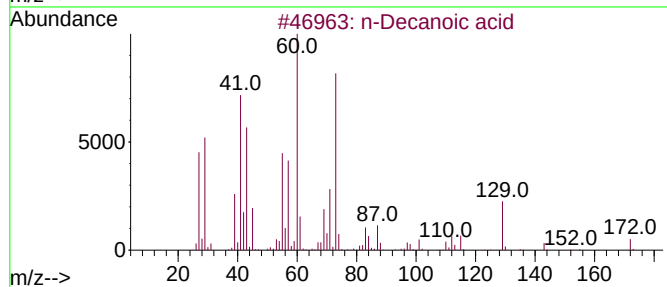
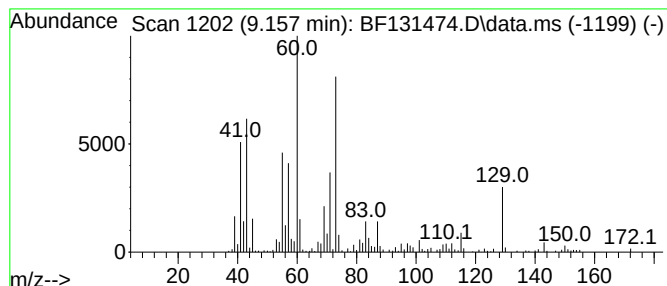
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Decanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	5.44 ng	233271	Acenaphthene-d10	10.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	91
2			Octanoic acid	144	C8H16O2	000124-07-2	64
3			Hexanoic acid	116	C6H12O2	000142-62-1	53
4			D-Fucose	164	C6H12O5	003615-37-0	53
5			Nonanoic acid	158	C9H18O2	000112-05-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131474.D
Acq On : 30 Nov 2022 16:41
Operator : CG\JU
Sample : N5799-01
Misc :
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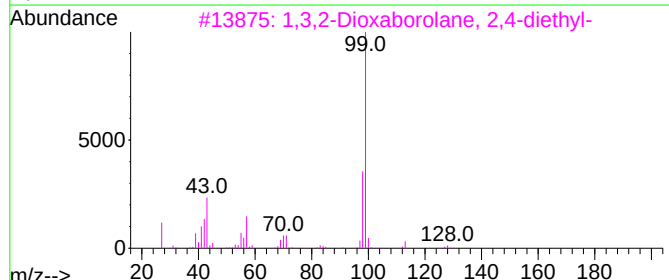
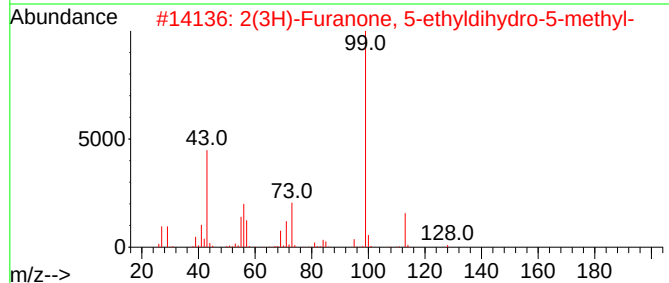
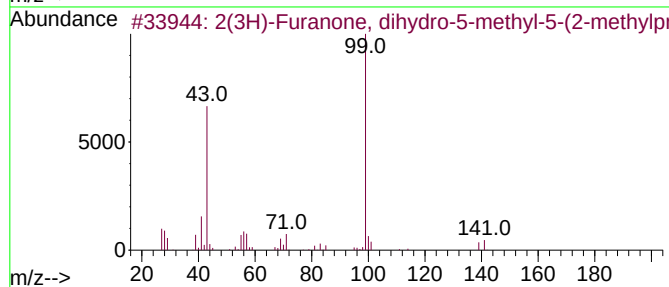
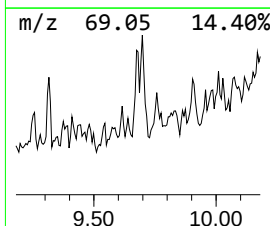
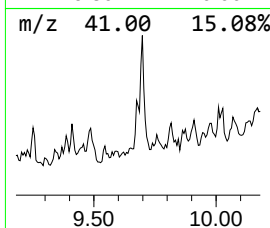
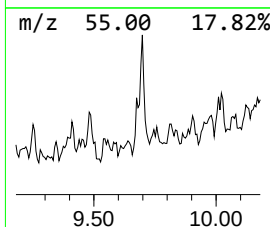
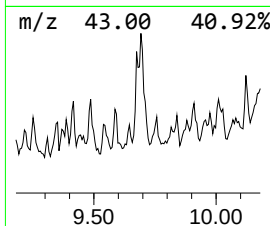
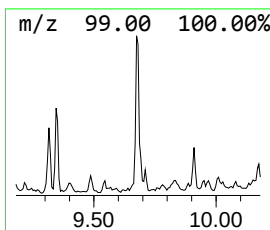
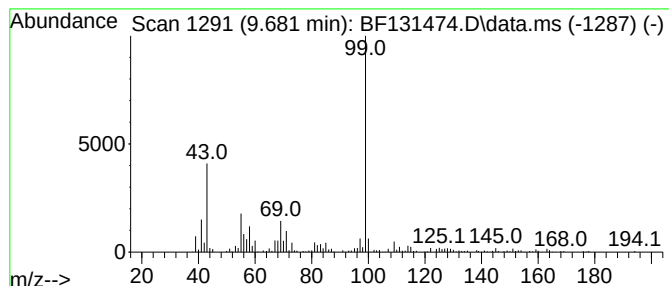
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2(3H)-Furanone, dihydro-5-m... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.681	3.93 ng	168528	Acenaphthene-d10		10.004	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-5-methyl...		156	C9H16O2	010200-21-2	64
2	2(3H)-Furanone, 5-ethyldihydro-5...		128	C7H12O2	002865-82-9	59
3	1,3,2-Dioxaborolane, 2,4-diethyl-		128	C6H13BO2	057633-63-3	59
4	Furan, 2,5-dihydro-2,5-dimethoxy-		130	C6H10O3	000332-77-4	58
5	Phosphoric acid, monododecyl ester		266	C12H27O4P	002627-35-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
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ClientSampleId :
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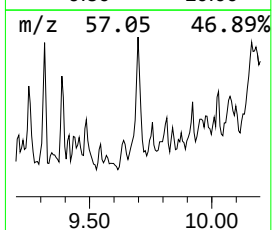
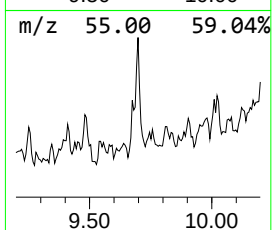
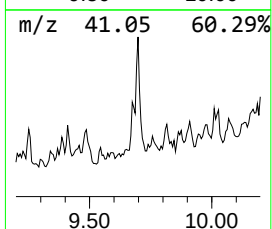
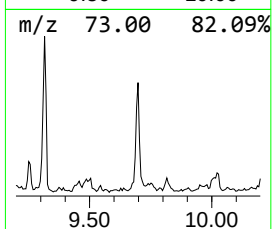
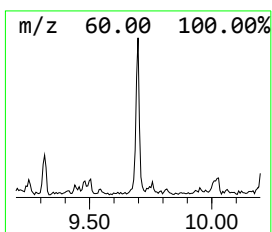
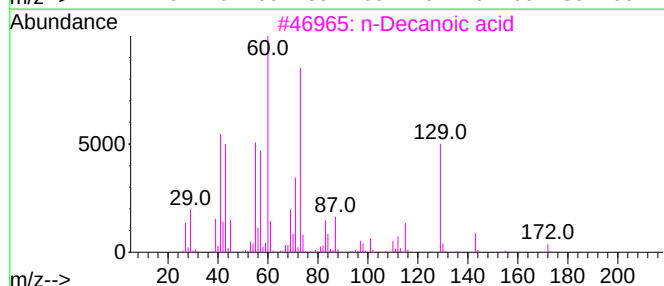
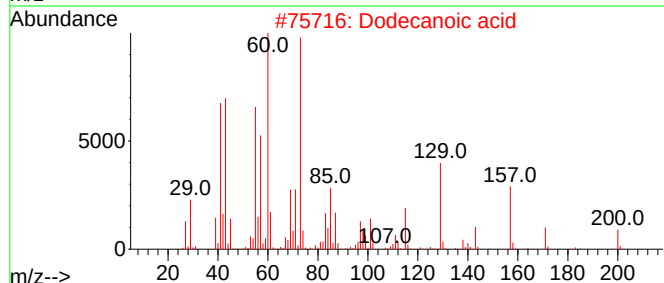
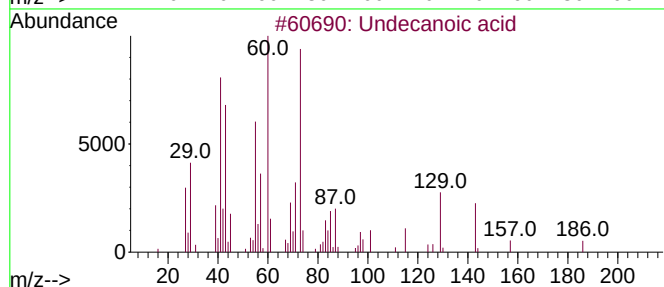
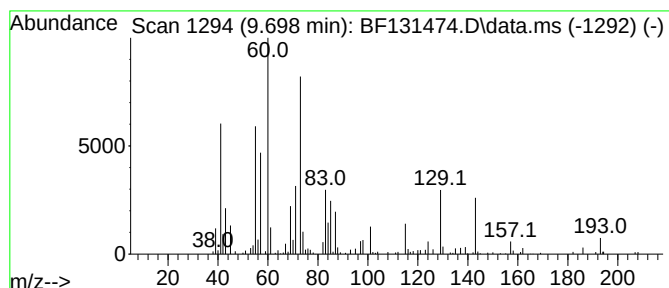
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.698	6.75 ng	289788	Acenaphthene-d10	10.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	93
2			Dodecanoic acid	200	C12H24O2	000143-07-7	64
3			n-Decanoic acid	172	C10H20O2	000334-48-5	53
4			Octanoic acid	144	C8H16O2	000124-07-2	49
5			Nonanoic acid	158	C9H18O2	000112-05-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131474.D
Acq On : 30 Nov 2022 16:41
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Sample : N5799-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
220-1-STONES

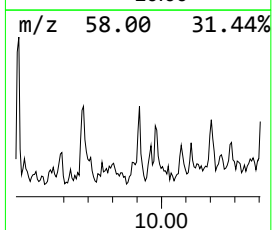
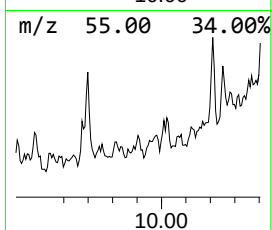
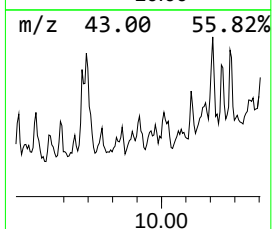
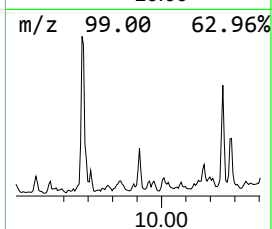
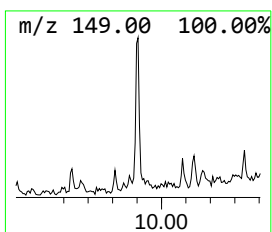
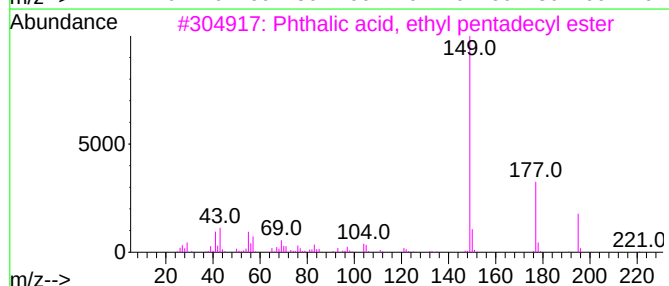
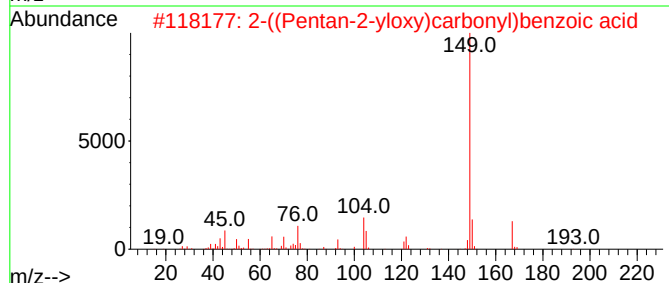
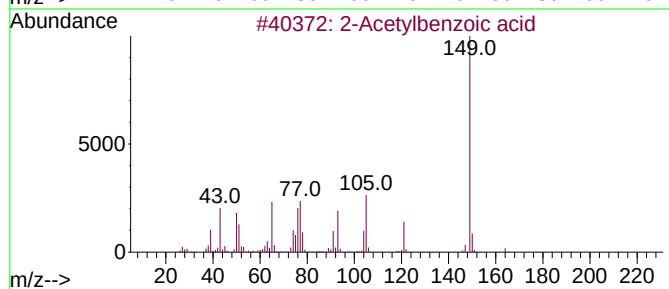
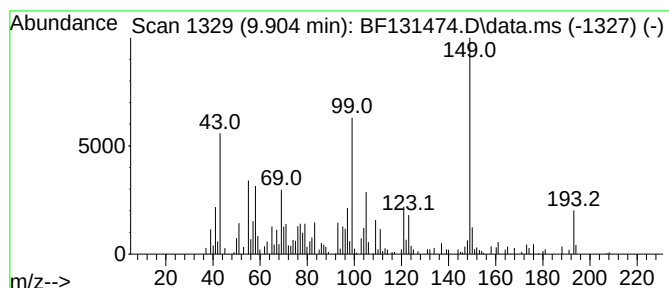
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown9.904 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.904	2.79 ng	119609	Acenaphthene-d10	10.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Acetylbenzoic acid	164	C9H8O3	000577-56-0	42
2			2-((Pentan-2-yloxy)carbonyl)benz...	236	C13H16O4	158703-44-7	35
3			Phthalic acid, ethyl pentadecyl ...	404	C25H40O4	1000308-93-3	35
4			1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	35
5			Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131474.D
Acq On : 30 Nov 2022 16:41
Operator : CG\JU
Sample : N5799-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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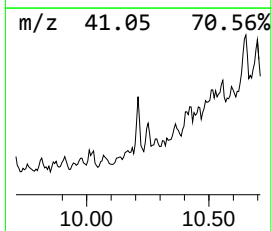
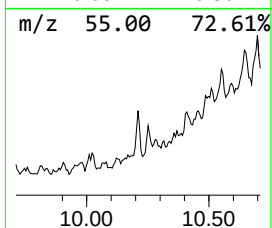
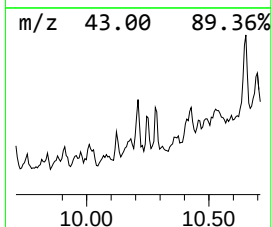
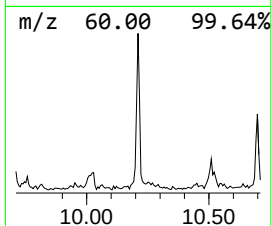
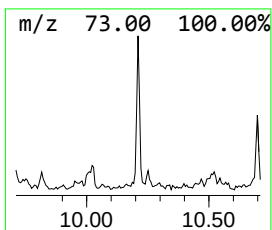
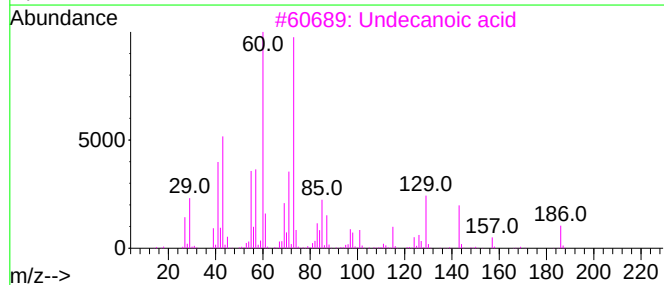
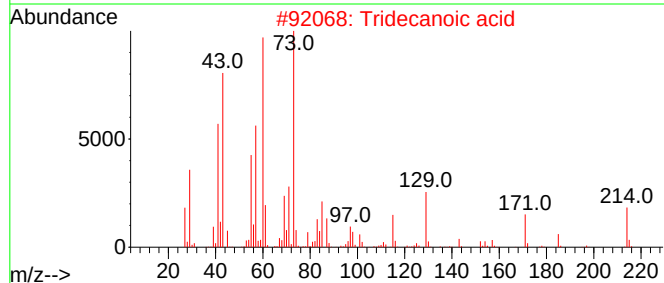
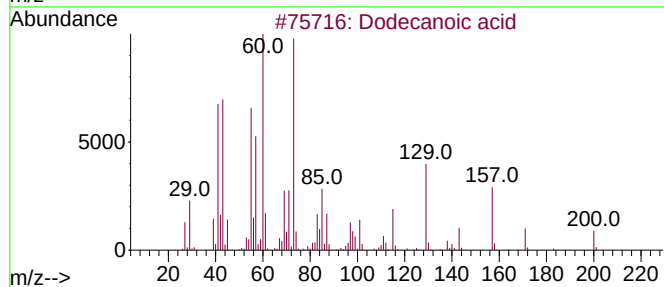
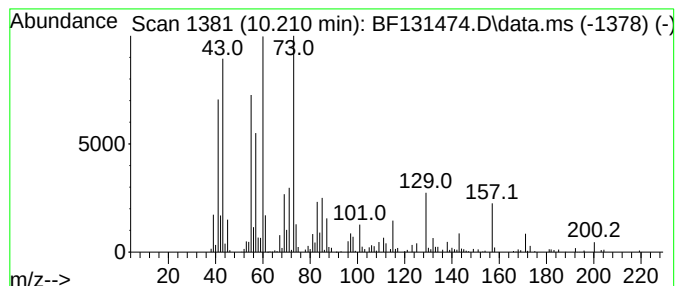
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.210	4.53 ng	194445	Acenaphthene-d10	10.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecanoic acid	200	C12H24O2	000143-07-7	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	80
3		Undecanoic acid	186	C11H22O2	000112-37-8	80
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		Nonanoic acid	158	C9H18O2	000112-05-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
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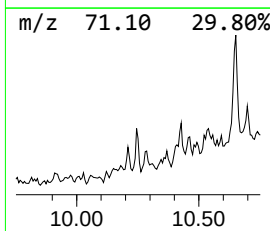
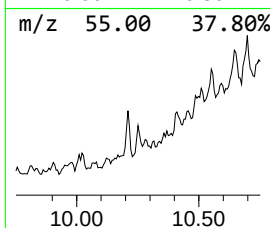
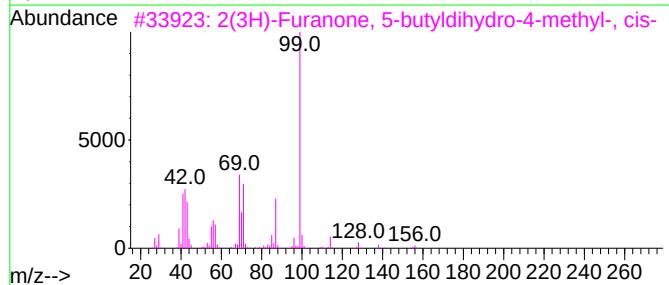
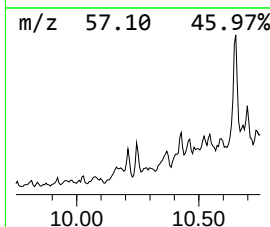
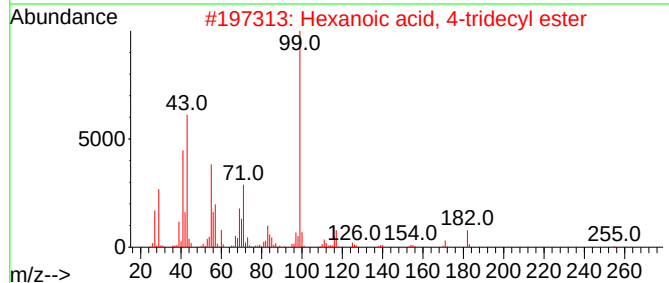
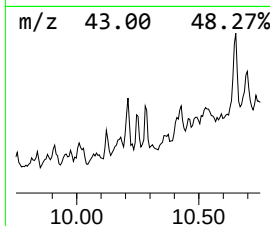
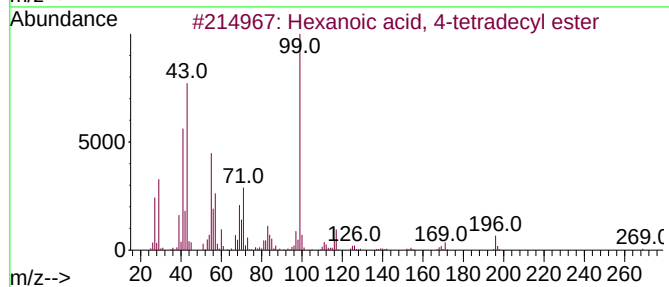
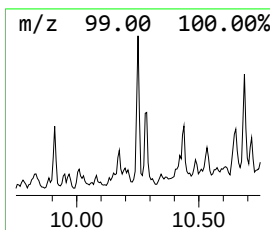
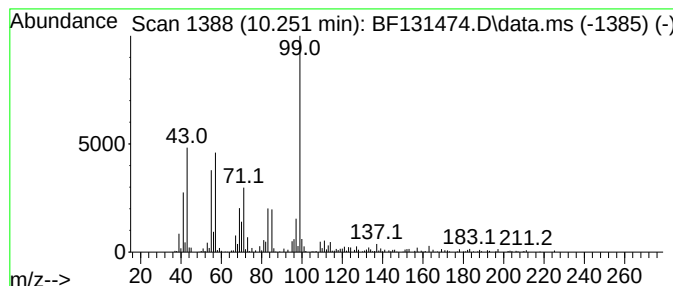
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Hexanoic acid, 4-tetradecyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.251	3.97 ng	170469	Acenaphthene-d10		10.004	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexanoic acid, 4-tetradecyl ester		312	C20H40O2	1000279-29-8	59
2	Hexanoic acid, 4-tridecyl ester		298	C19H38O2	1000279-29-3	53
3	2(3H)-Furanone, 5-butyldihydro-4...		156	C9H16O2	055013-32-6	50
4	trans-3-Methyl-4-octanolide		156	C9H16O2	039638-67-0	49
5	Furan, 2,5-dihydro-2,5-dimethoxy-		130	C6H10O3	000332-77-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
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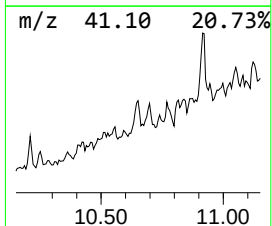
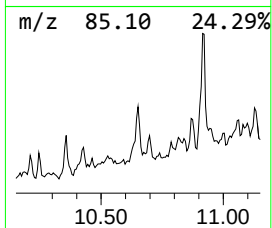
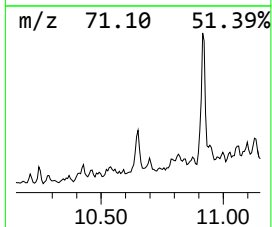
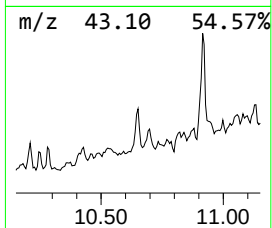
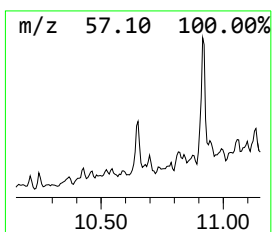
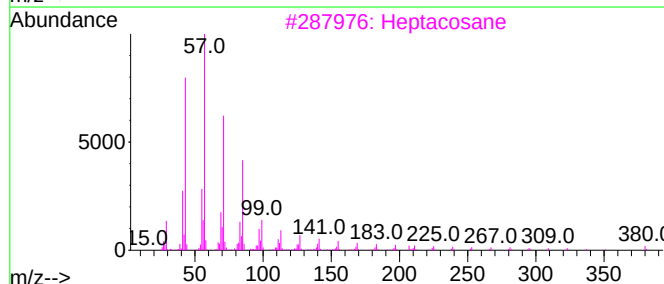
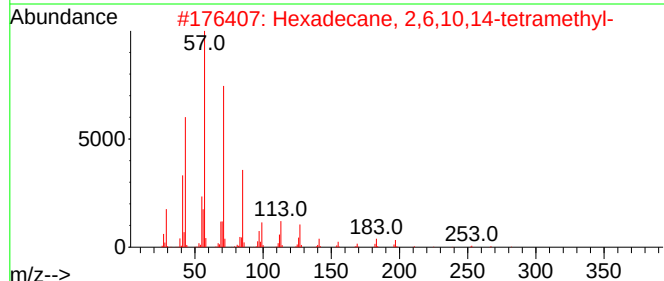
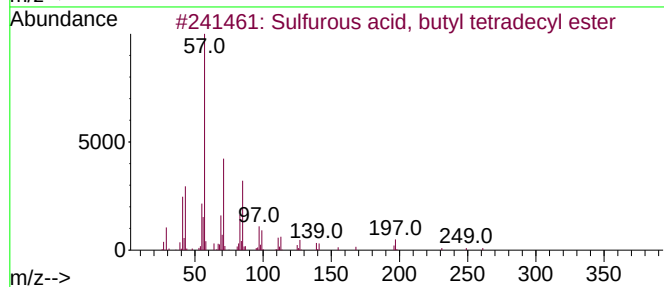
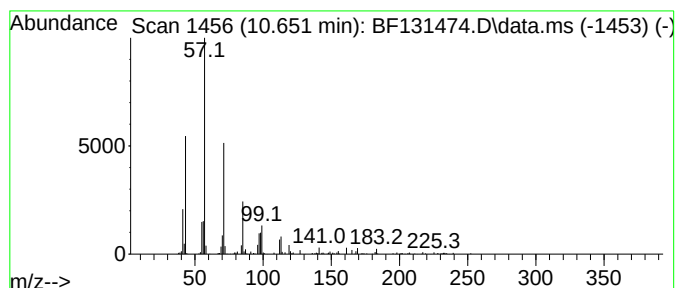
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Sulfurous acid, butyl tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.651	4.89 ng	209896	Acenaphthene-d10		10.004	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tetradecyl...		334	C18H38O3S	1010309-18-1	64
2	Hexadecane, 2,6,10,14-tetramethyl-		282	C20H42	000638-36-8	64
3	Heptacosane		380	C27H56	000593-49-7	59
4	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	59
5	Nonadecane, 2-methyl-		282	C20H42	001560-86-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131474.D
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Misc :
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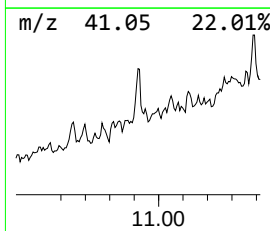
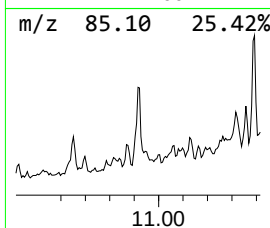
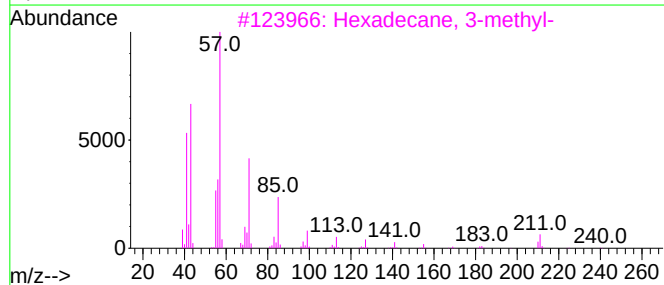
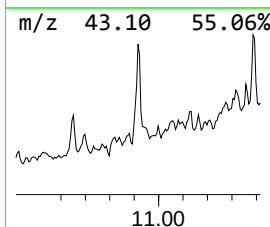
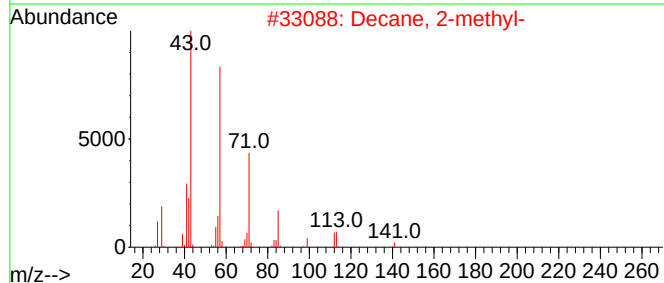
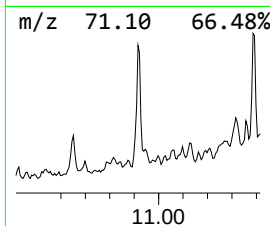
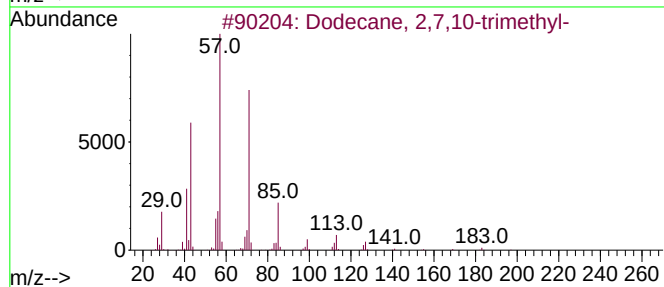
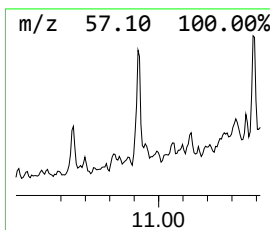
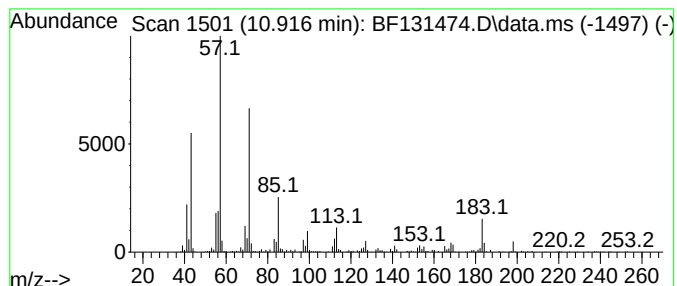
Instrument :
BNA_F
ClientSampleId :
220-1-STONES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Dodecane, 2,7,10-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.916	18.87 ng	862783	Phenanthrene-d10		11.504	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-		212	C15H32	074645-98-0	68
2	Decane, 2-methyl-		156	C11H24	006975-98-0	68
3	Hexadecane, 3-methyl-		240	C17H36	006418-43-5	62
4	Dodecane, 2,6,11-trimethyl-		212	C15H32	031295-56-4	58
5	Heptacosane		380	C27H56	000593-49-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131474.D
Acq On : 30 Nov 2022 16:41
Operator : CG\JU
Sample : N5799-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

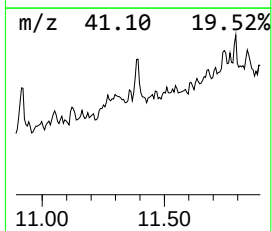
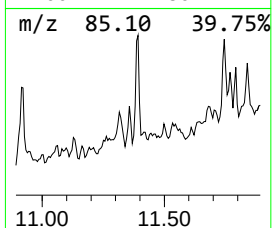
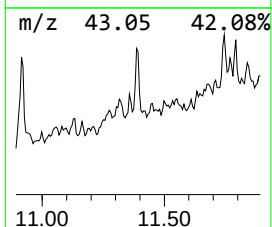
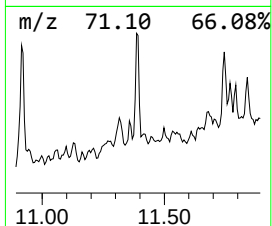
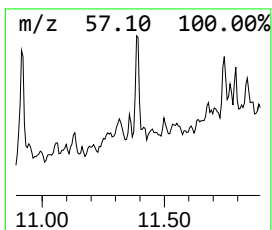
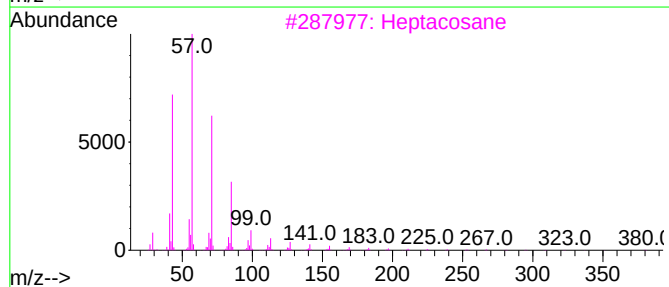
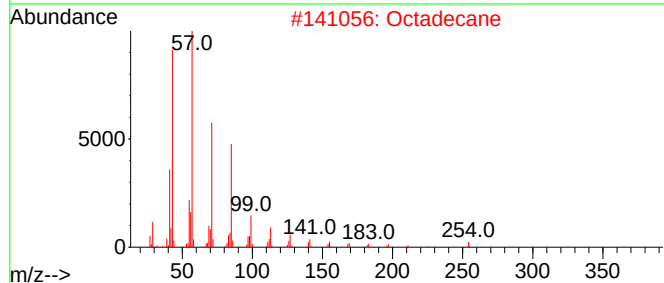
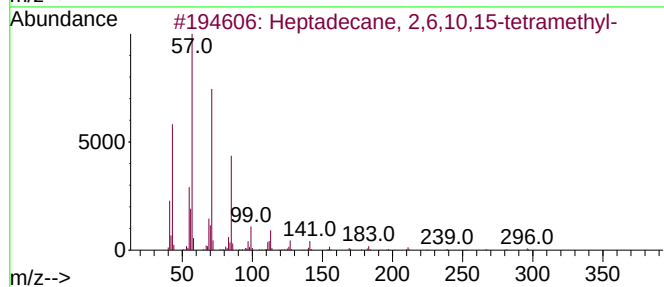
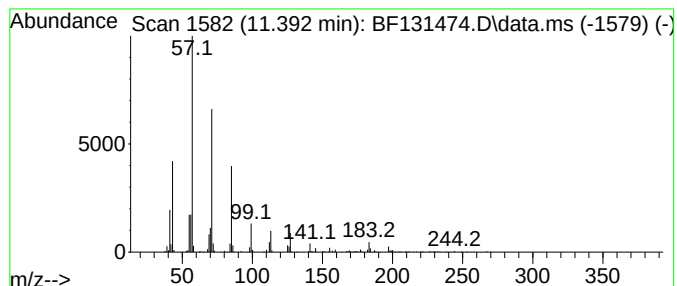
Instrument :
BNA_F
ClientSampleId :
220-1-STONES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Heptadecane, 2,6,10,15-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.392	15.03 ng	687581	Phenanthrene-d10		11.504	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	90
2	Octadecane		254	C18H38	000593-45-3	90
3	Heptacosane		380	C27H56	000593-49-7	90
4	Tridecane, 2-methyl-		198	C14H30	001560-96-9	87
5	2-Bromotetradecane		276	C14H29Br	074036-95-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131474.D
Acq On : 30 Nov 2022 16:41
Operator : CG\JU
Sample : N5799-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
220-1-STONES

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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...	2.252	23.4	ng	670326	1	6.945	571781	20.0
3-Penten-2-one,...	4.551	2.8	ng	79698	1	6.945	571781	20.0
2-Pentanone, 4-...	5.175	60.5	ng	1730650	1	6.945	571781	20.0
2-Pentanone, 4-...	5.957	4.4	ng	126085	1	6.945	571781	20.0
unknown6.657	6.657	2.9	ng	81520	1	6.945	571781	20.0
unknown7.140	7.140	3.3	ng	95389	1	6.945	571781	20.0
Heptanoic acid	7.304	3.0	ng	85785	1	6.945	571781	20.0
Ethanol, 2-(2-b...	8.139	6.0	ng	247208	2	8.234	817511	20.0
Nonanoic acid	8.592	7.6	ng	309831	2	8.234	817511	20.0
unknown8.651	8.651	3.5	ng	145188	2	8.234	817511	20.0
n-Decanoic acid	9.157	5.4	ng	233271	3	10.004	858166	20.0
2(3H)-Furanone,...	9.681	3.9	ng	168528	3	10.004	858166	20.0
Undecanoic acid	9.698	6.8	ng	289788	3	10.004	858166	20.0
unknown9.904	9.904	2.8	ng	119609	3	10.004	858166	20.0
Dodecanoic acid	10.210	4.5	ng	194445	3	10.004	858166	20.0
Hexanoic acid, ...	10.251	4.0	ng	170469	3	10.004	858166	20.0
Sulfurous acid,...	10.651	4.9	ng	209896	3	10.004	858166	20.0
Dodecane, 2,7,1...	10.916	18.9	ng	862783	4	11.504	914660	20.0
Heptadecane, 2,...	11.392	15.0	ng	687581	4	11.504	914660	20.0