

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
 Data File : BF138369.D
 Acq On : 27 Jun 2024 16:37
 Operator : CG\JU
 Sample : P3049-01 10X
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SHOP-RAG-DRUM

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-BF061224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138369.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	4	9	16	rVB	303771	366004	5.75%	0.718%
2	2.492	50	69	72	rBV5	81854	477868	7.50%	0.937%
3	3.951	312	317	332	rVB	729723	1267827	19.91%	2.487%
4	5.469	571	575	580	rVV2	240721	298166	4.68%	0.585%
5	5.516	580	583	589	rVB	285754	308655	4.85%	0.605%
6	5.722	616	618	626	rVV2	149553	195334	3.07%	0.383%
7	5.786	626	629	634	rVB	310814	277681	4.36%	0.545%
8	5.904	646	649	652	rVB	114733	109608	1.72%	0.215%
9	6.039	667	672	675	rVB3	100264	147943	2.32%	0.290%
10	6.128	684	687	693	rVB3	222233	311179	4.89%	0.610%
11	6.316	714	719	721	rBV2	131007	167449	2.63%	0.328%
12	6.375	727	729	731	rVB	193782	134006	2.10%	0.263%
13	6.404	731	734	737	rBV	665977	584656	9.18%	1.147%
14	6.433	737	739	742	rVB	212177	165976	2.61%	0.326%
15	6.463	742	744	746	rBV	212784	237422	3.73%	0.466%
16	6.528	752	755	758	rBV	236706	310357	4.87%	0.609%
17	6.563	759	761	766	rVB	206083	192362	3.02%	0.377%
18	6.616	766	770	775	rBV4	110545	210387	3.30%	0.413%
19	6.710	782	786	789	rBV2	938366	1187831	18.65%	2.330%
20	6.880	810	815	818	rVV	1529175	1508542	23.69%	2.959%
21	6.933	821	824	828	rVV2	431181	477163	7.49%	0.936%
22	6.986	831	833	836	rVV2	97101	106720	1.68%	0.209%
23	7.022	836	839	843	rVV2	244271	276837	4.35%	0.543%
24	7.057	843	845	847	rVV	238148	178267	2.80%	0.350%
25	7.127	855	857	858	rVV	170198	137870	2.16%	0.270%
26	7.151	858	861	864	rVV	481062	414208	6.50%	0.813%
27	7.198	864	869	870	rVV2	373863	453292	7.12%	0.889%
28	7.216	870	872	875	rVV2	177803	162836	2.56%	0.319%
29	7.269	875	881	884	rVV3	303909	445674	7.00%	0.874%
30	7.339	891	893	895	rBV	162214	143314	2.25%	0.281%
31	7.363	895	897	900	rVB	164598	125416	1.97%	0.246%
32	7.410	900	905	907	rBV2	403736	394164	6.19%	0.773%
33	7.433	907	909	913	rVV2	334673	458031	7.19%	0.899%
34	7.469	913	915	919	rVB	736415	611097	9.59%	1.199%
35	7.527	919	925	927	rBV3	330287	547037	8.59%	1.073%
36	7.657	927	947	949	rVV	1538502	6368979	100.00%	12.494%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
 Data File : BF138369.D
 Acq On : 27 Jun 2024 16:37
 Operator : CG\JU
 Sample : P3049-01 10X
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SHOP-RAG-DRUM

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-BF061224.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	7.680	949	951	953	rVV2	279438	346122	5.43%	0.679%
38	7.704	953	955	958	rVV	819087	606384	9.52%	1.190%
39	7.763	960	965	966	rBV2	107982	120065	1.89%	0.236%
40	7.780	966	968	970	rVV2	169644	164017	2.58%	0.322%
41	7.798	970	971	975	rVV3	175186	227487	3.57%	0.446%
42	7.833	975	977	981	rVV3	252181	299953	4.71%	0.588%
43	7.874	981	984	986	rVV2	179656	200051	3.14%	0.392%
44	7.898	986	988	995	rVV5	369402	609867	9.58%	1.196%
45	7.951	995	997	999	rVV	142893	120107	1.89%	0.236%
46	7.998	1003	1005	1008	rVB	282044	203909	3.20%	0.400%
47	8.063	1013	1016	1020	rBV	255521	266708	4.19%	0.523%
48	8.139	1020	1029	1030	rBV	623676	725814	11.40%	1.424%
49	8.163	1030	1033	1035	rVV	1865197	1739997	27.32%	3.413%
50	8.216	1038	1042	1044	rVB2	206518	256400	4.03%	0.503%
51	8.357	1063	1066	1067	rBV	133308	119881	1.88%	0.235%
52	8.380	1067	1070	1072	rVV	1049551	925320	14.53%	1.815%
53	8.404	1072	1074	1078	rVV	1269149	982958	15.43%	1.928%
54	8.451	1078	1082	1085	rVV5	138578	192485	3.02%	0.378%
55	8.504	1088	1091	1094	rVV3	86372	106930	1.68%	0.210%
56	8.539	1094	1097	1100	rVV3	126890	140472	2.21%	0.276%
57	8.574	1100	1103	1105	rVV3	140987	121252	1.90%	0.238%
58	8.663	1114	1118	1121	rBV	267478	237718	3.73%	0.466%
59	8.745	1129	1132	1136	rBV	480121	369376	5.80%	0.725%
60	8.816	1141	1144	1146	rVV2	118321	115283	1.81%	0.226%
61	8.857	1146	1151	1155	rVV	3616816	3097985	48.64%	6.077%
62	8.886	1155	1156	1161	rVB	299050	255328	4.01%	0.501%
63	8.980	1167	1172	1174	rBV2	134803	153370	2.41%	0.301%
64	9.110	1190	1194	1198	rVB3	87244	122342	1.92%	0.240%
65	9.227	1211	1214	1217	rBV	610391	515386	8.09%	1.011%
66	9.310	1224	1228	1231	rBV	494267	391127	6.14%	0.767%
67	9.563	1265	1271	1274	rBV5	139763	230722	3.62%	0.453%
68	9.627	1278	1282	1285	rVV4	134878	193733	3.04%	0.380%
69	9.657	1285	1287	1291	rVV4	91372	144190	2.26%	0.283%
70	9.768	1303	1306	1311	rVB3	261250	303468	4.76%	0.595%
71	9.839	1315	1318	1321	rVB	463385	327511	5.14%	0.642%
72	9.910	1327	1330	1334	rBV	2106723	1760772	27.65%	3.454%
73	10.016	1344	1348	1352	rVB	123553	141888	2.23%	0.278%
74	10.063	1352	1356	1360	rBV	974211	946288	14.86%	1.856%
75	10.286	1390	1394	1397	rVV	879807	808056	12.69%	1.585%
76	10.339	1400	1403	1405	rVB	274438	201667	3.17%	0.396%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
 Data File : BF138369.D
 Acq On : 27 Jun 2024 16:37
 Operator : CG\JU
 Sample : P3049-01 10X
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SHOP-RAG-DRUM

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-BF061224.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	10.815	1481	1484	1488	rVB2	144374	181701	2.85%	0.356%
78	11.015	1516	1518	1520	rVV	216654	200110	3.14%	0.393%
79	11.080	1524	1529	1533	rVV	155151	220270	3.46%	0.432%
80	11.121	1533	1536	1541	rVV	116139	150295	2.36%	0.295%
81	11.398	1579	1583	1586	rBV	1802673	1478556	23.21%	2.900%
82	11.739	1637	1641	1645	rVB2	125307	152224	2.39%	0.299%
83	11.780	1645	1648	1655	rVB4	106941	135450	2.13%	0.266%
84	11.868	1656	1663	1666	rBV	69895	116550	1.83%	0.229%
85	11.915	1666	1671	1677	rBV	241523	297650	4.67%	0.584%
86	12.092	1698	1701	1706	rVB2	85829	109084	1.71%	0.214%
87	12.580	1780	1784	1787	rBV2	101355	109767	1.72%	0.215%
88	12.639	1791	1794	1797	rVB	712001	554342	8.70%	1.087%
89	12.733	1807	1810	1816	rBV	179667	231949	3.64%	0.455%
90	12.786	1816	1819	1822	rVB	183005	150289	2.36%	0.295%
91	12.939	1841	1845	1848	rVV	5364142	4515317	70.90%	8.858%
92	12.980	1848	1852	1859	rVB	388084	427419	6.71%	0.838%
93	13.474	1933	1936	1942	rVB	132756	121951	1.91%	0.239%
94	13.880	2002	2005	2014	rVB	135139	147719	2.32%	0.290%
95	14.033	2027	2031	2037	rBV	1566106	1327505	20.84%	2.604%
96	14.415	2093	2096	2099	rVB2	189136	170142	2.67%	0.334%
97	14.503	2107	2111	2117	rVB	137779	165995	2.61%	0.326%
98	14.803	2159	2162	2169	rVB	188559	263277	4.13%	0.516%
99	15.150	2218	2221	2228	rVB	103992	129120	2.03%	0.253%
100	15.503	2276	2281	2285	rBV	885059	1067989	16.77%	2.095%

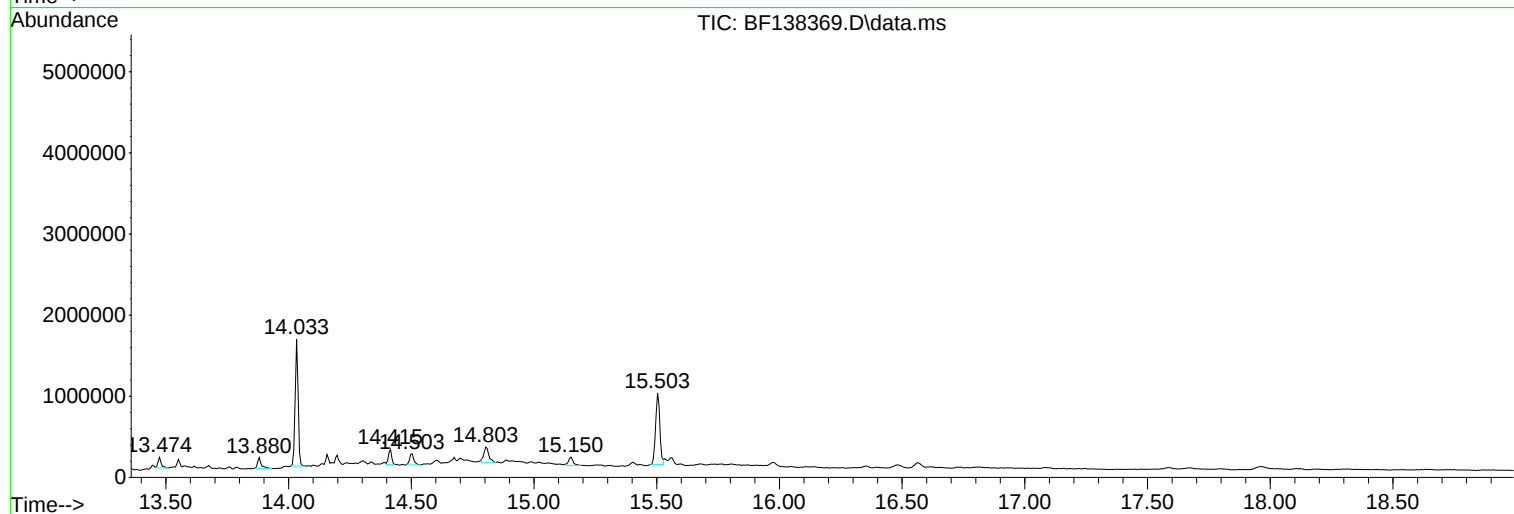
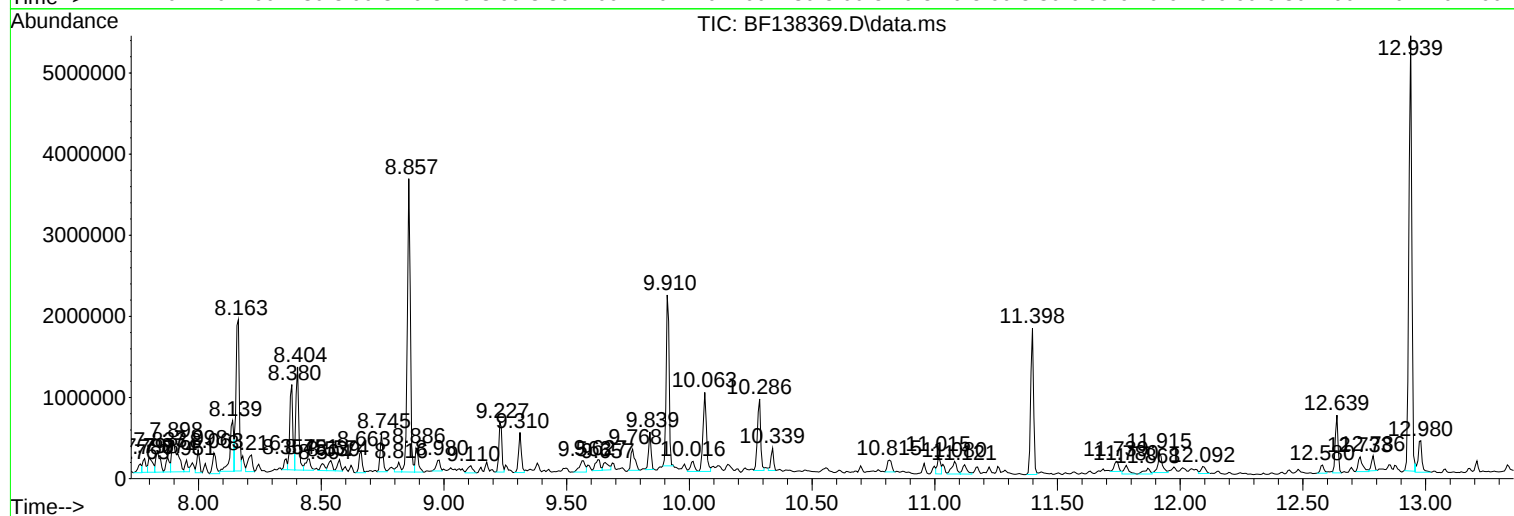
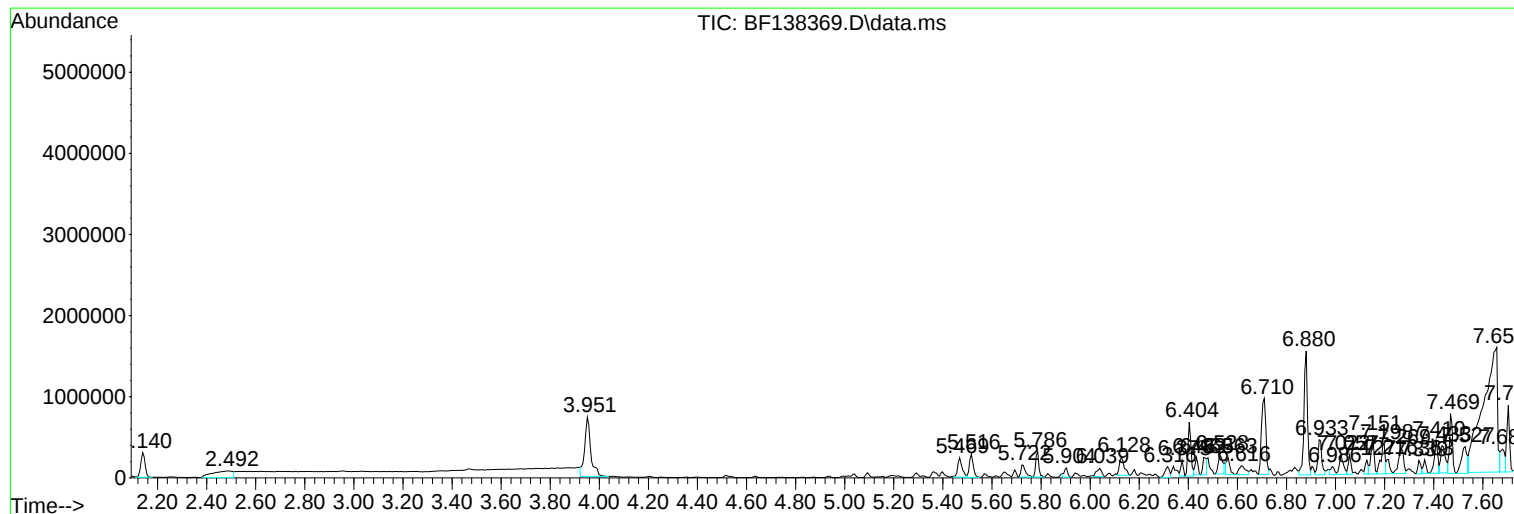
Sum of corrected areas: 50977218

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

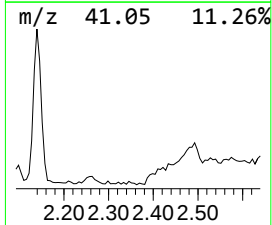
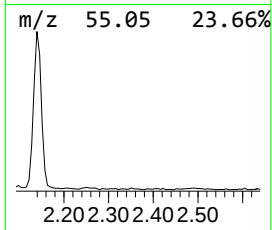
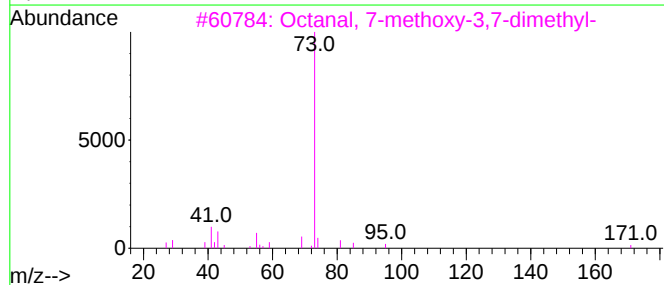
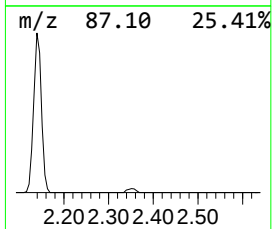
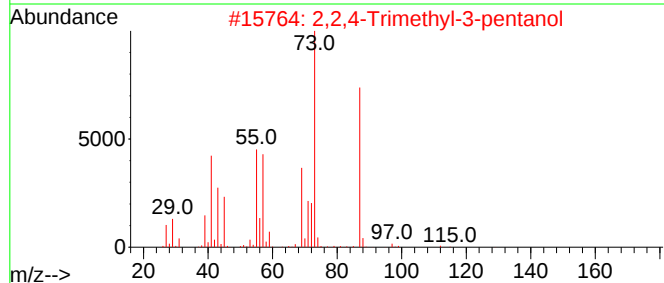
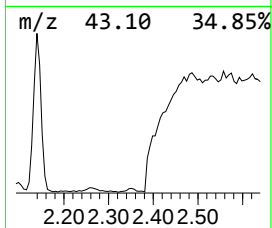
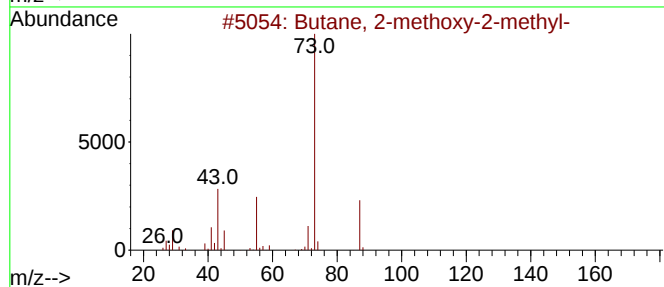
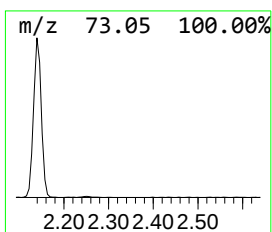
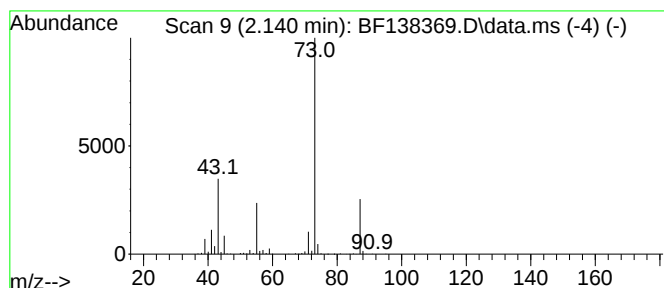
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	4.85 ng	366004	1,4-Dichlorobenzene-d4	6.880

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			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	23
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

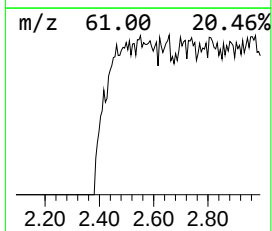
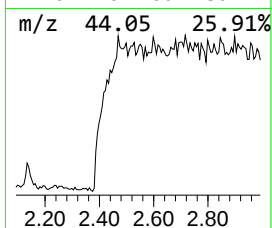
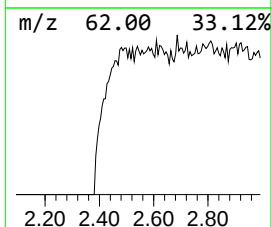
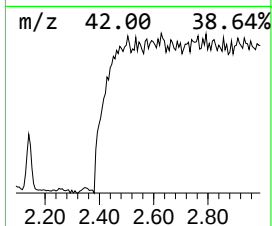
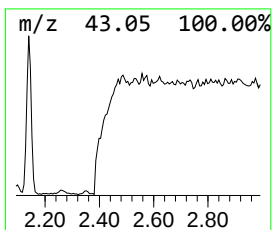
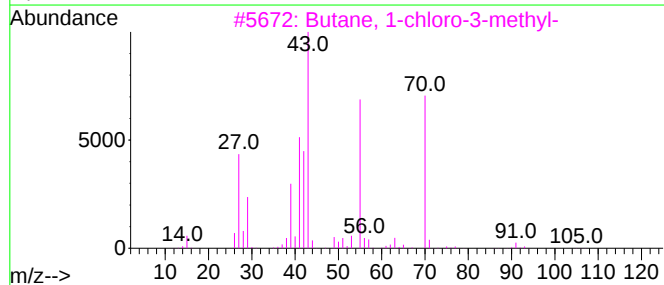
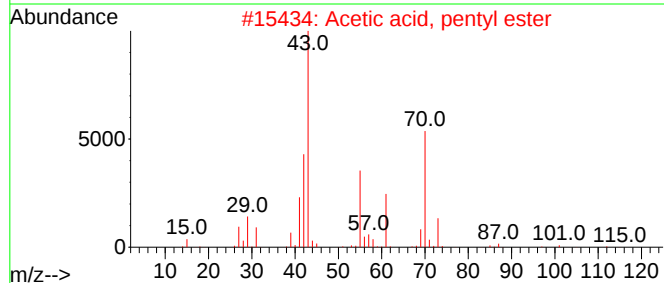
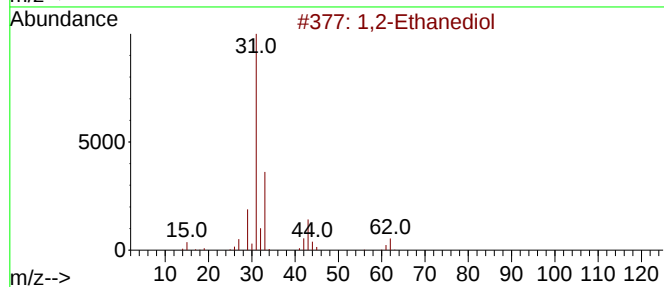
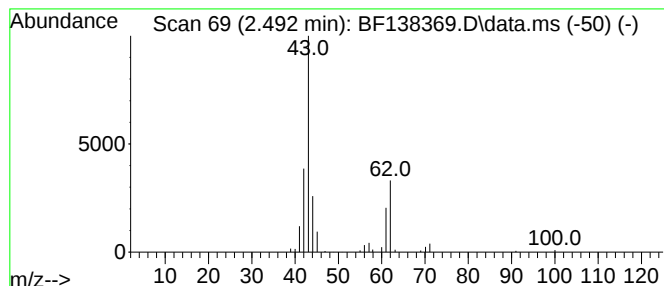
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown2.492 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.492	6.34 ng	477868	1,4-Dichlorobenzene-d4	6.880

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Ethanediol	62	C2H6O2	000107-21-1	42
2		Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9
3		Butane, 1-chloro-3-methyl-	106	C5H11Cl	000107-84-6	9
4		Ethanethiol	62	C2H6S	000075-08-1	5
5		Ethene, chloro-	62	C2H3Cl	000075-01-4	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

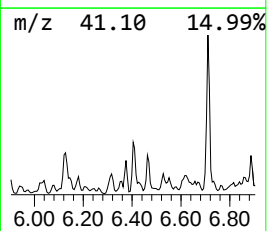
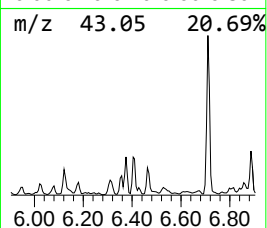
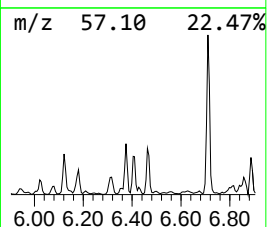
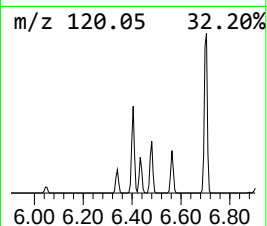
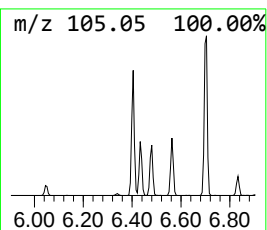
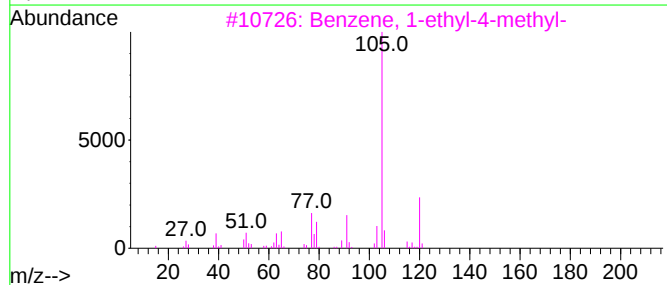
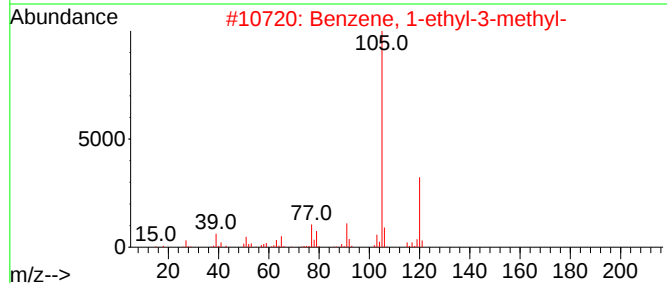
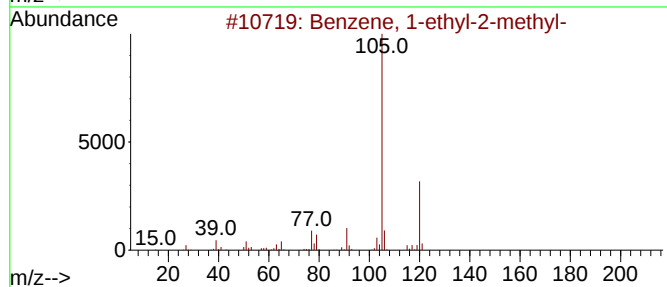
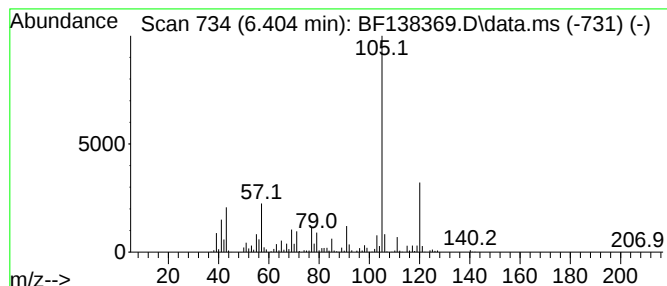
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.404	7.75 ng	584656	1,4-Dichlorobenzene-d4	6.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4			Mesitylene	120	C9H12	000108-67-8	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

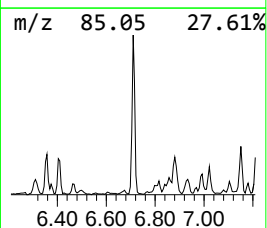
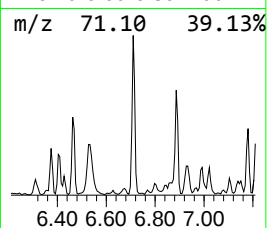
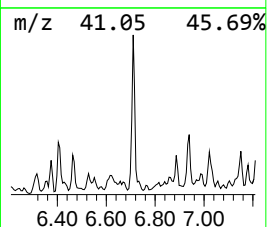
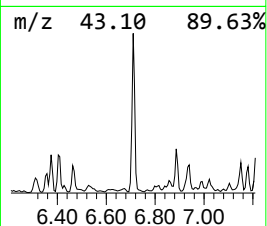
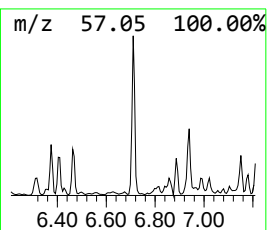
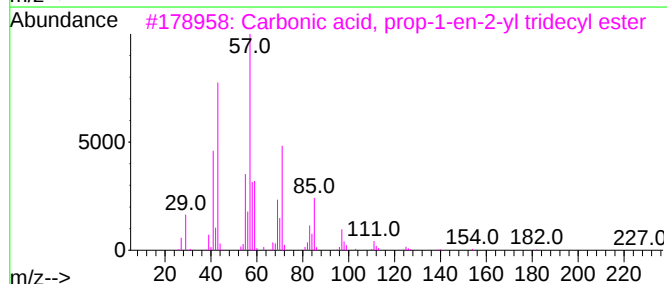
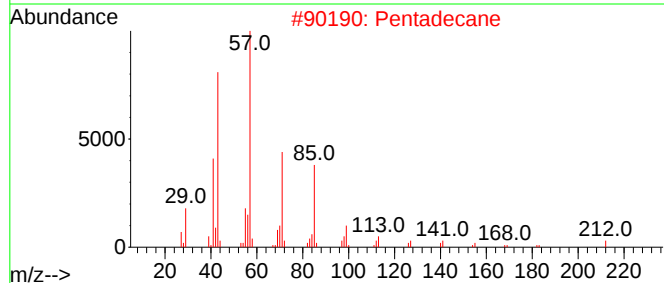
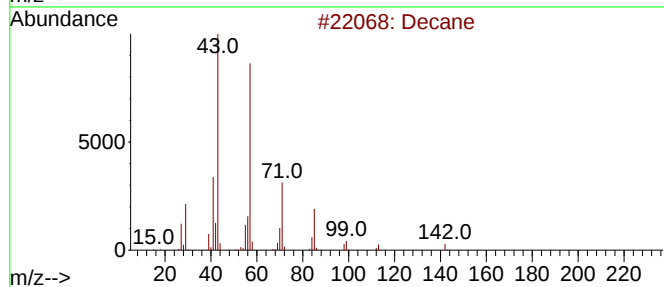
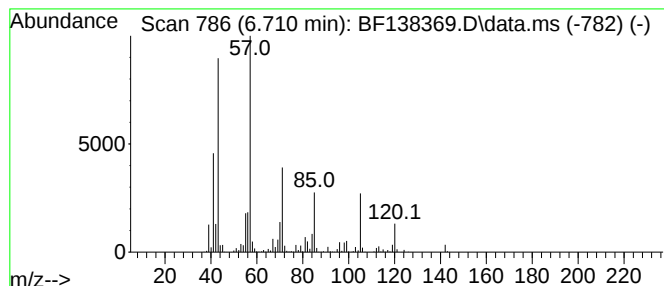
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Decane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.710	15.75 ng	1187830	1,4-Dichlorobenzene-d4	6.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	64
2			Pentadecane	212	C15H32	000629-62-9	59
3			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	59
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	50
5			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

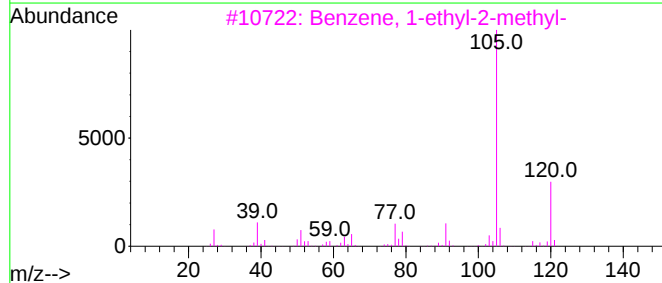
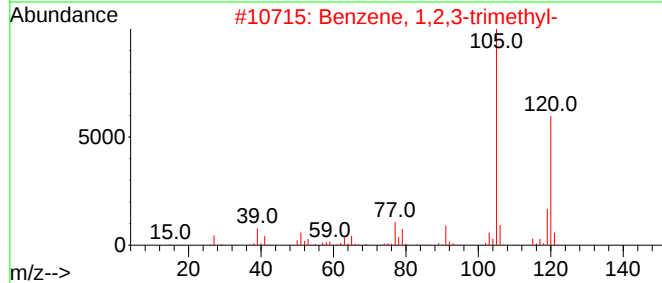
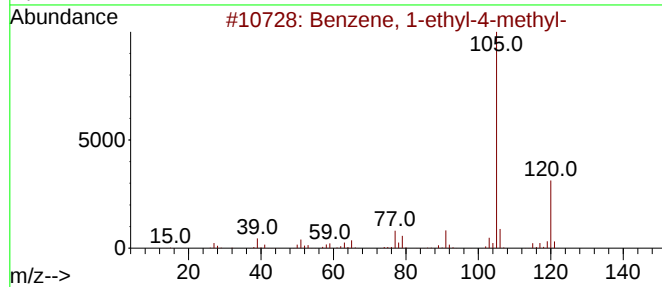
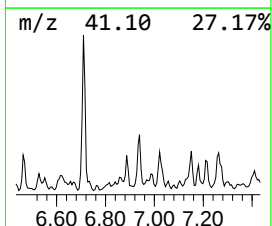
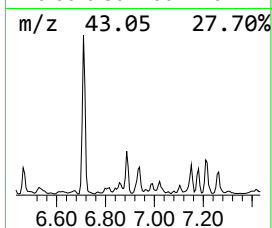
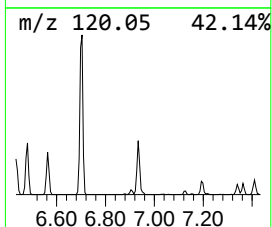
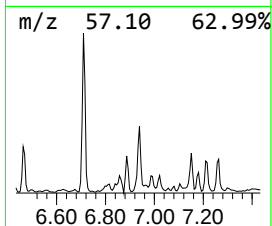
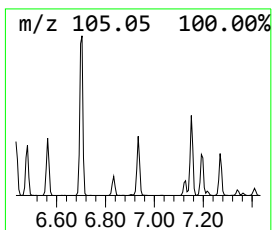
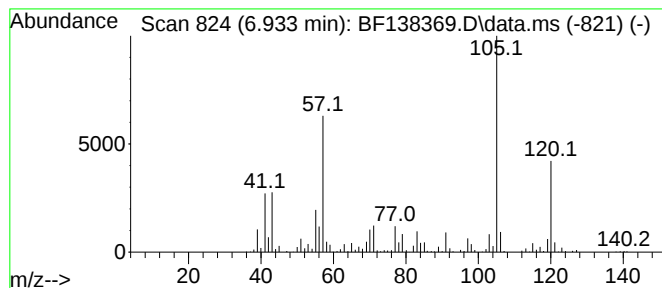
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1-ethyl-4-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.933	6.33 ng	477163	1,4-Dichlorobenzene-d4	6.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

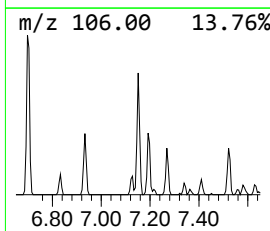
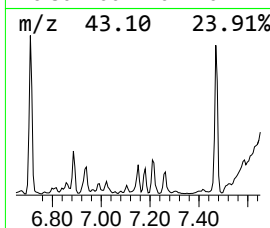
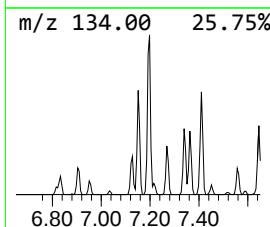
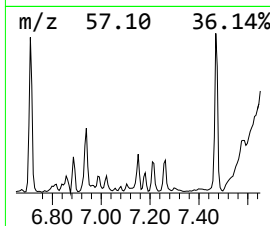
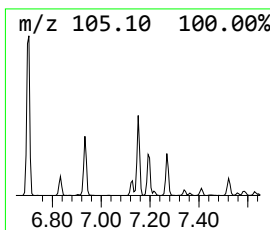
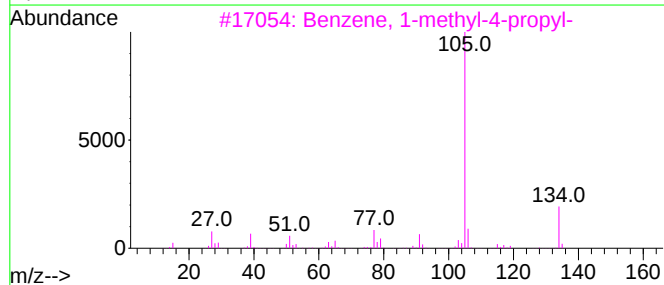
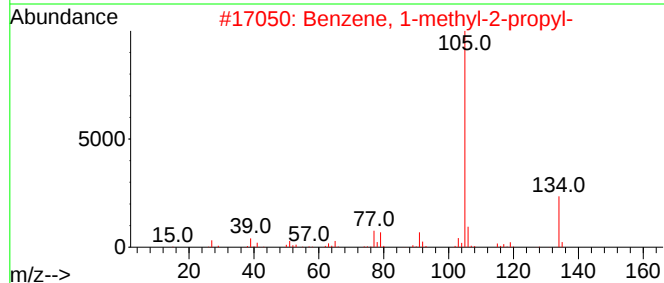
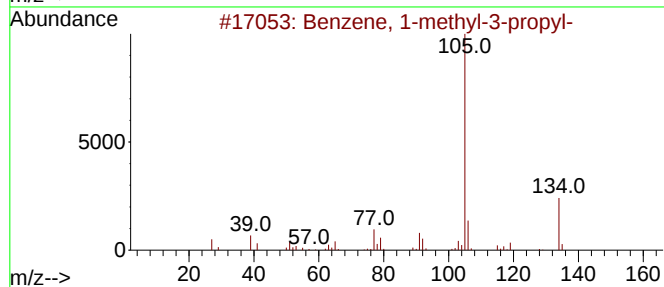
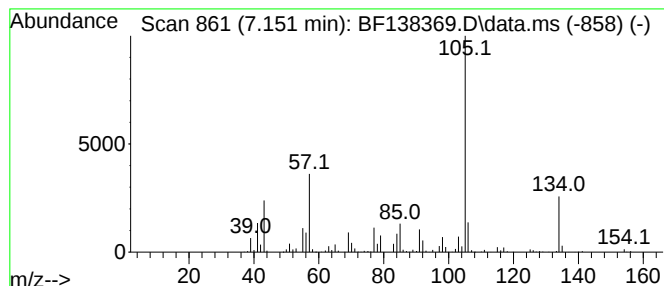
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, 1-methyl-3-propyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.151	5.49 ng	414208	1,4-Dichlorobenzene-d4	6.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	93
2			Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	81
3			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	76
4			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	68
5			2-Tolylloxirane	134	C9H10O	002783-26-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

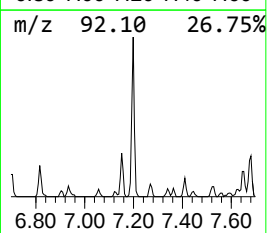
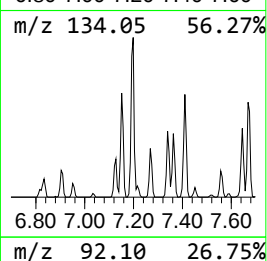
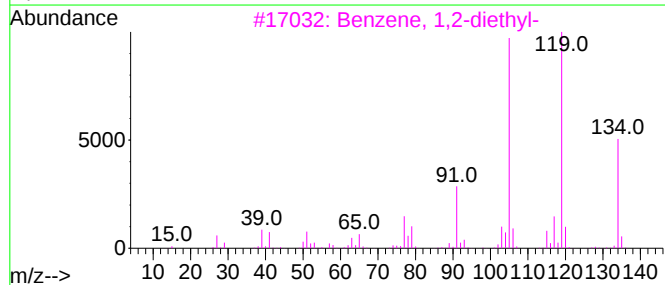
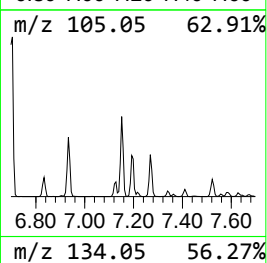
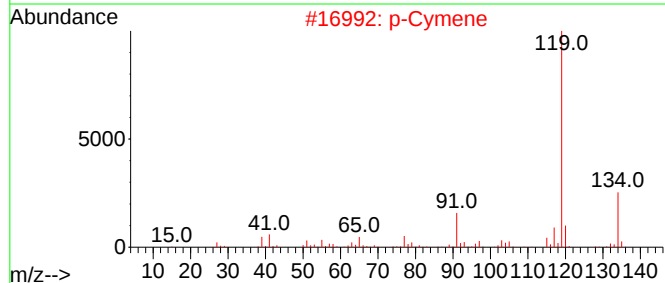
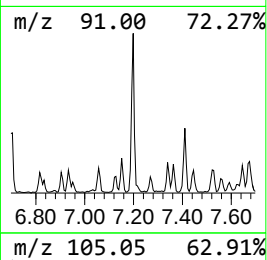
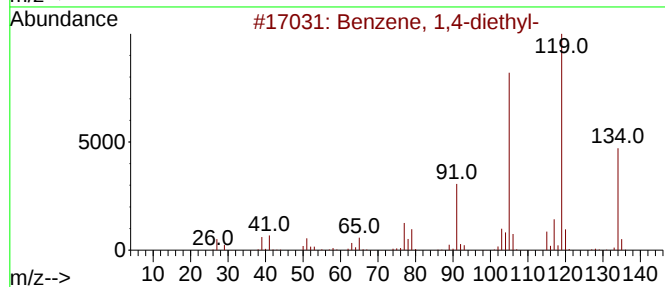
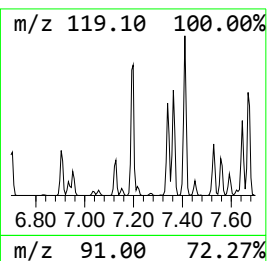
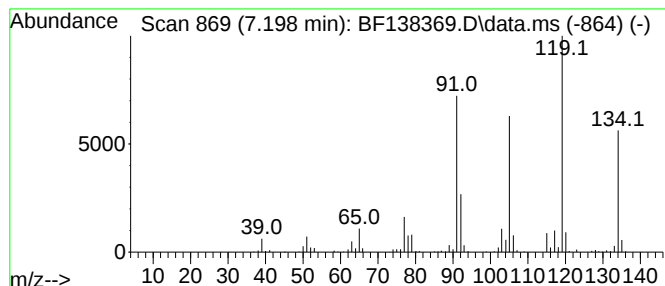
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, 1,4-diethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.198	6.01 ng	453292	1,4-Dichlorobenzene-d4	6.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	94
2			p-Cymene	134	C10H14	000099-87-6	93
3			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	93
4			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	92
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

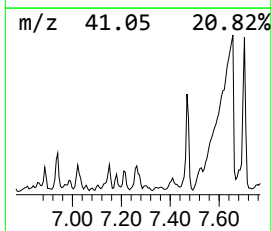
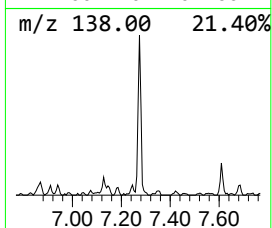
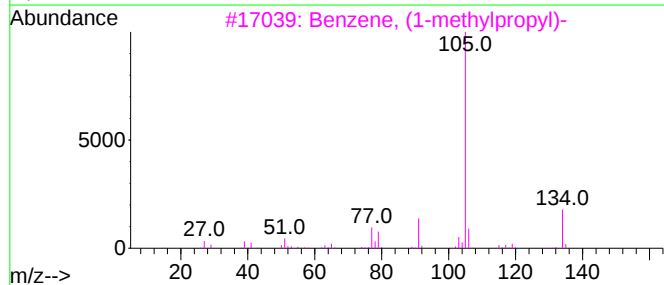
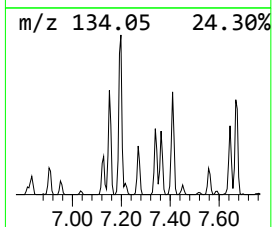
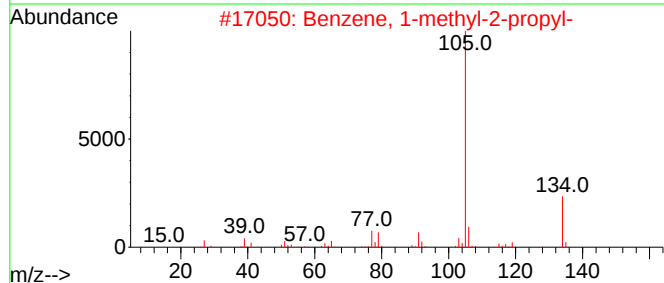
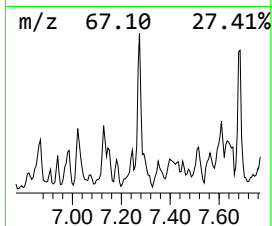
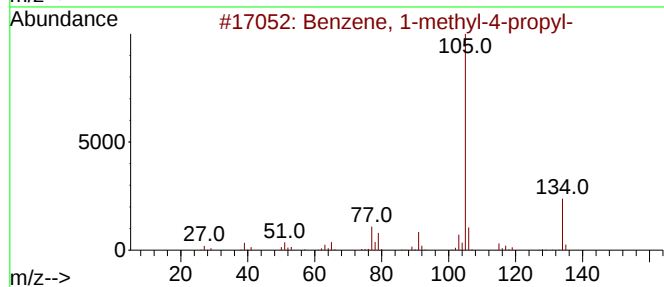
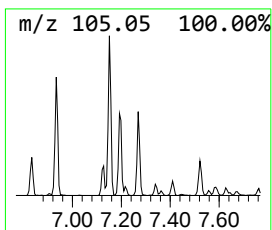
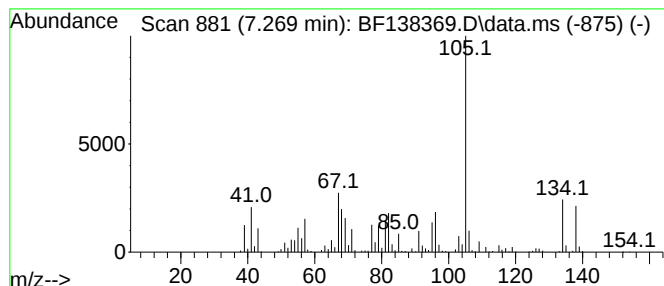
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzene, 1-methyl-4-propyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.269	5.91 ng	445674	1,4-Dichlorobenzene-d4	6.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	83
2			Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	80
3			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	42
4			3,4-Dimethylthiophenol	138	C8H10S	018800-53-8	42
5			Benzeneacetaldehyde, .alpha.-met...	134	C9H10O	000093-53-8	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

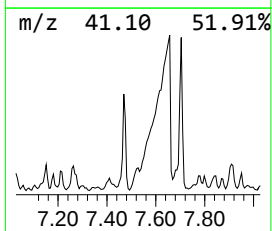
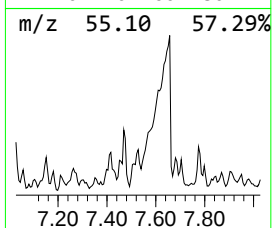
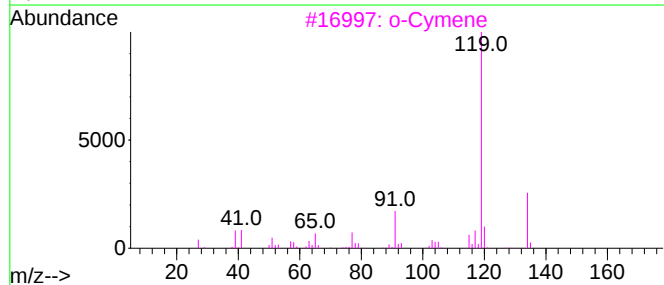
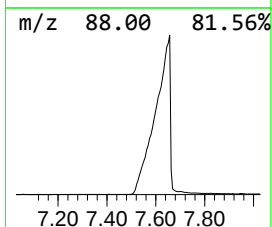
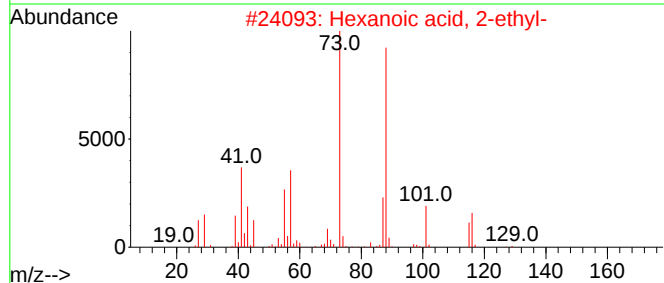
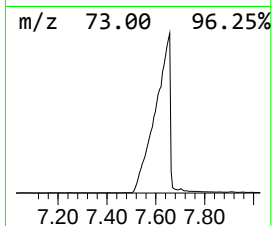
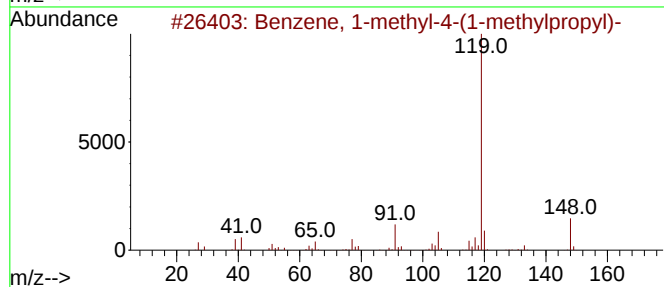
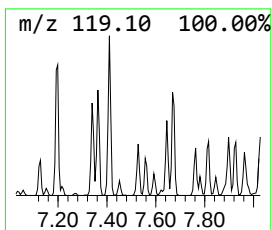
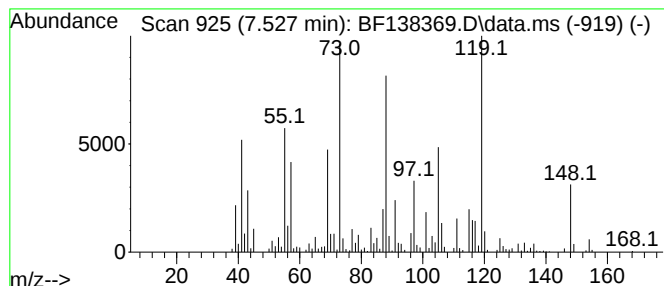
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown7.527 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.527	6.29 ng	547037	Naphthalene-d8	8.163

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	38
2		Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	38
3		o-Cymene	134	C10H14	000527-84-4	30
4		(+)-2-(Ethylamino)-3-phenylpropa...	179	C11H17NO	148260-44-0	27
5		p-Cymene	134	C10H14	000099-87-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

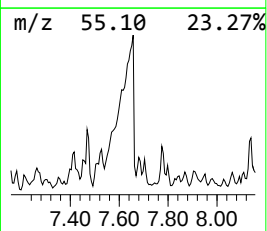
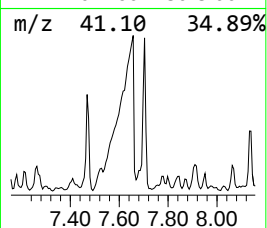
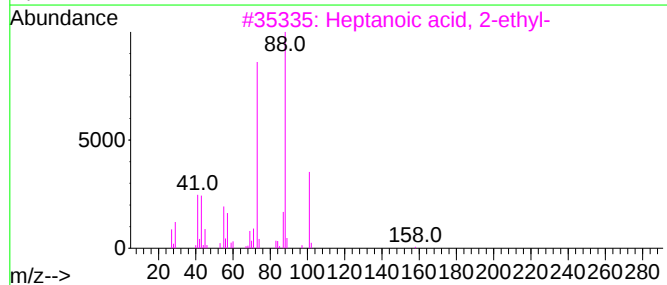
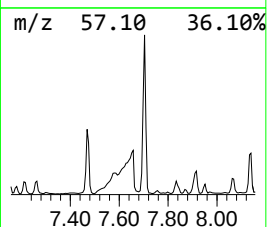
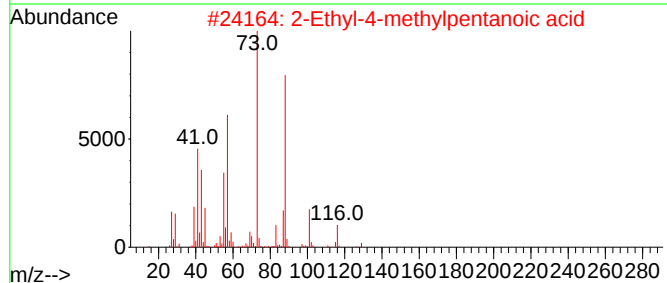
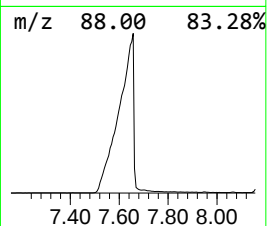
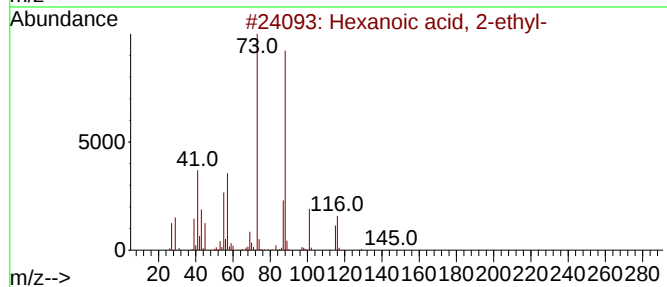
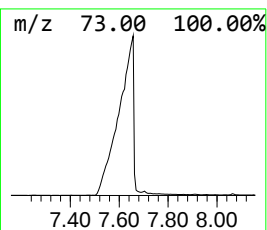
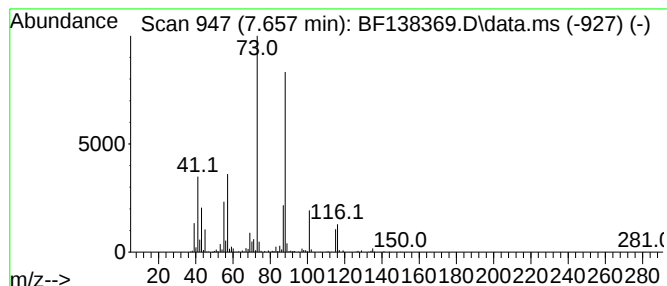
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.657	73.21 ng	6368980	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	91
2			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	64
3			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
4			Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	50
5			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

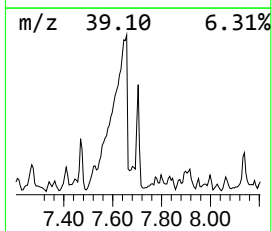
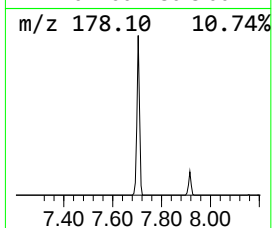
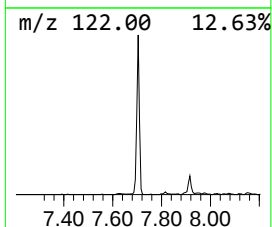
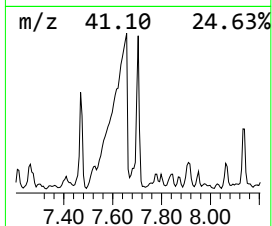
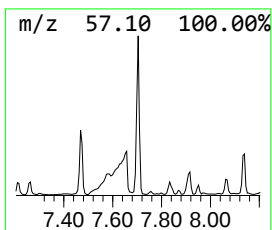
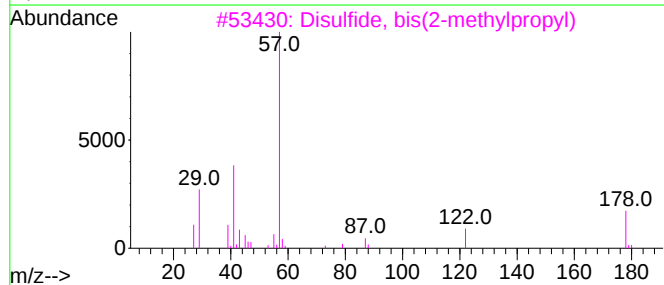
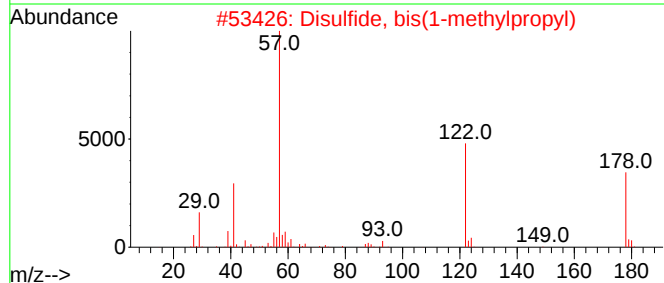
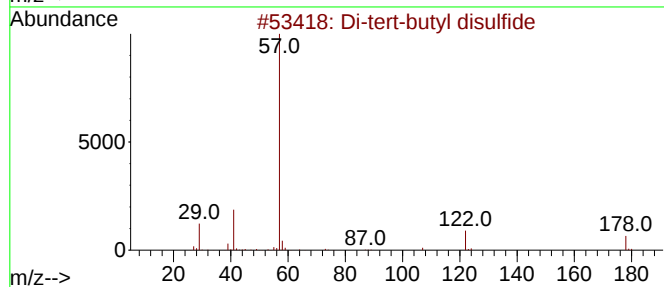
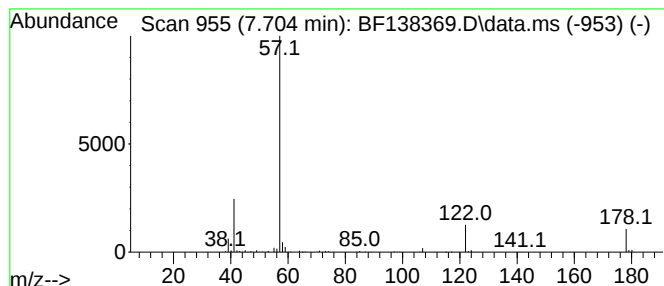
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Di-tert-butyl disulfide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.704	6.97 ng	606384	Naphthalene-d8	8.163

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	91
2		Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	59
3		Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	56
4		Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	23
5		Acetic acid, [(1,1-dimethylethyl...	148	C6H12O2S	024310-22-3	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

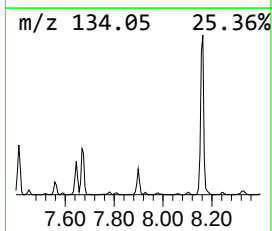
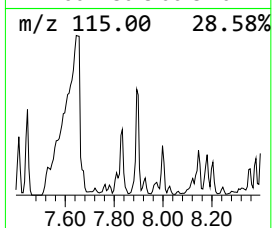
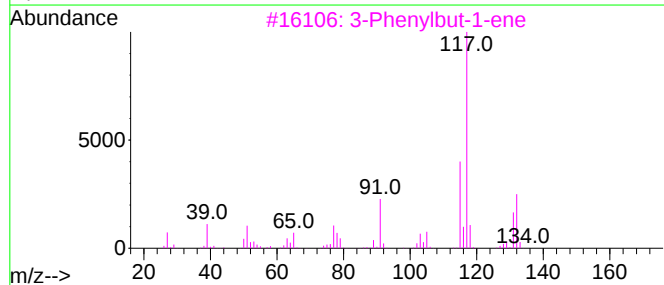
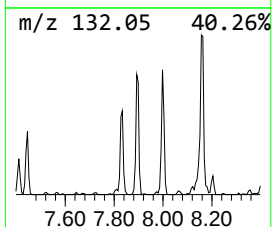
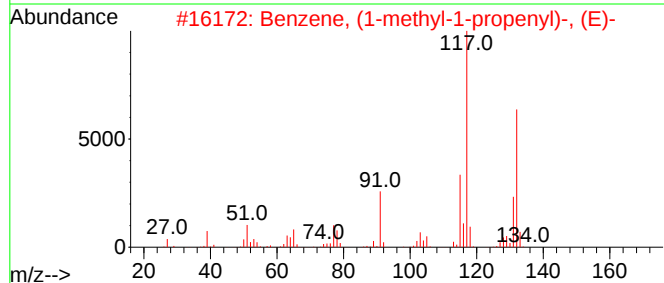
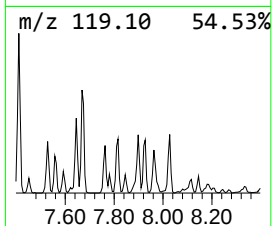
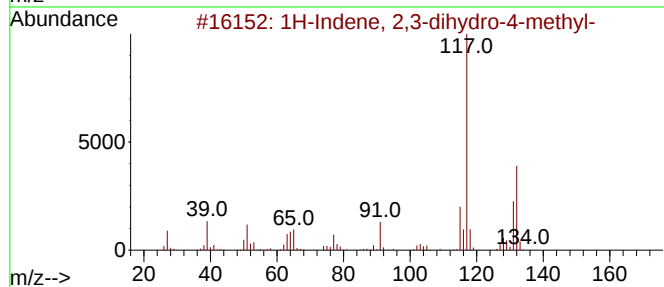
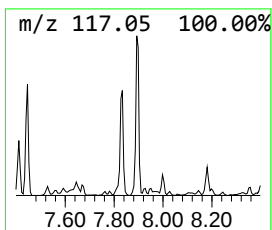
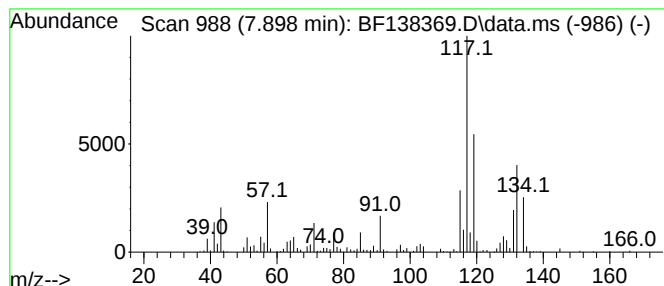
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.898	7.01 ng	609867	Naphthalene-d8	8.163

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12		000824-22-6	70
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12		000768-00-3	70
3	3-Phenylbut-1-ene	132	C10H12		000934-10-1	70
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12		000874-35-1	64
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12		003290-53-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

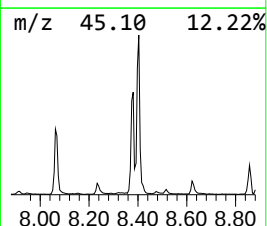
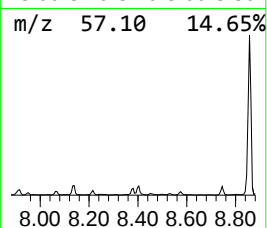
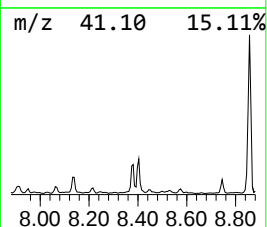
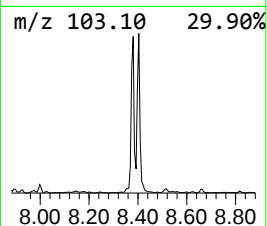
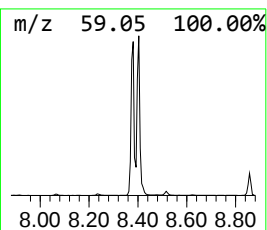
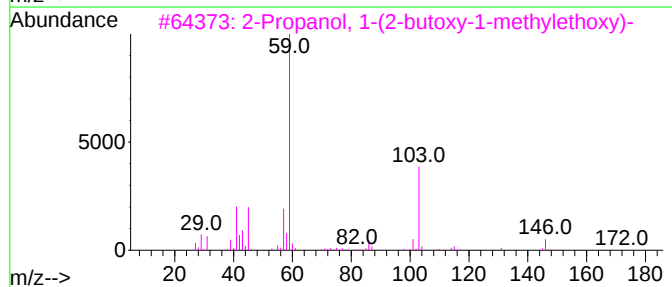
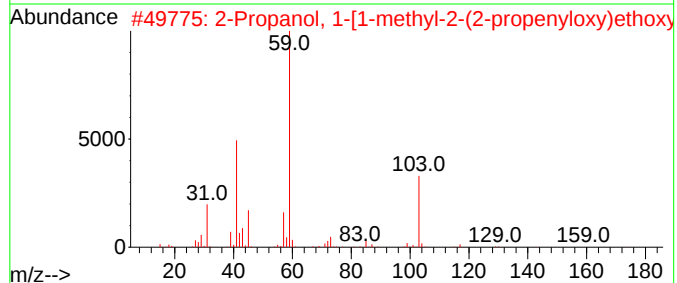
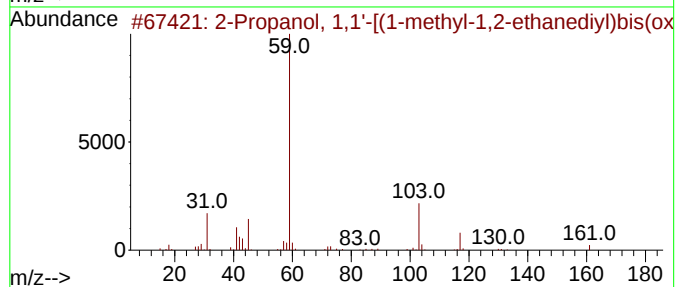
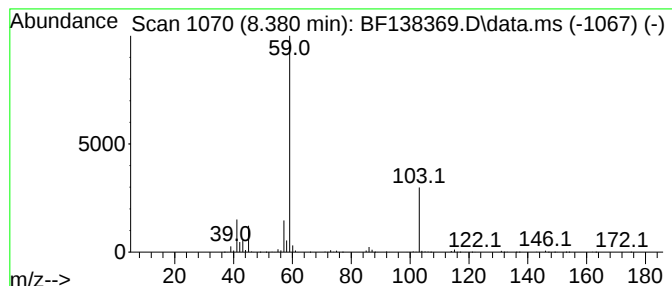
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2-Propanol, 1,1'-[(1-methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.380	10.64 ng	925320	Naphthalene-d8	8.163

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	78	
2	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78	
3	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74	
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72	
5	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1000367-13-2	59	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

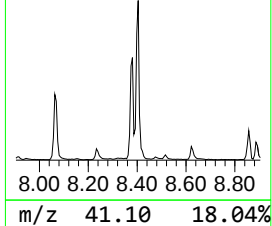
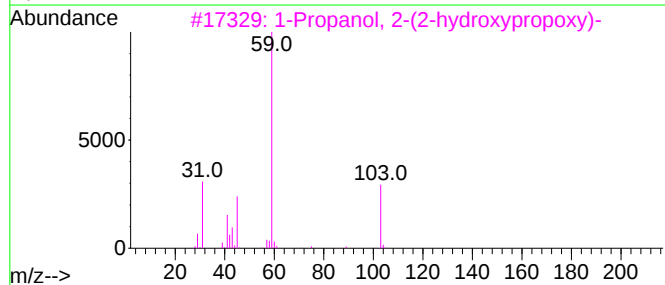
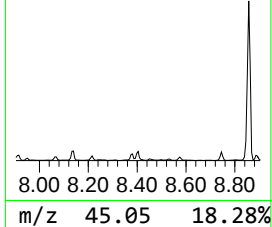
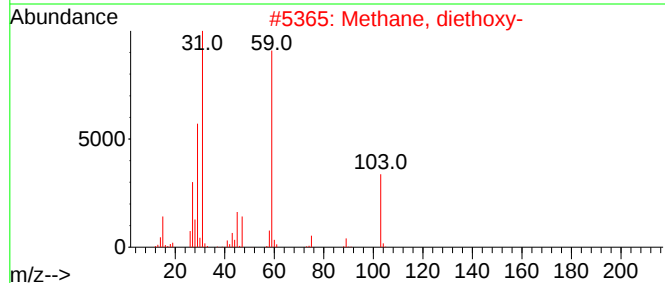
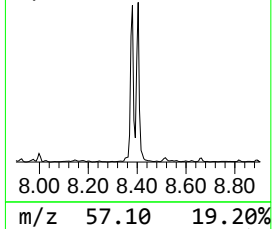
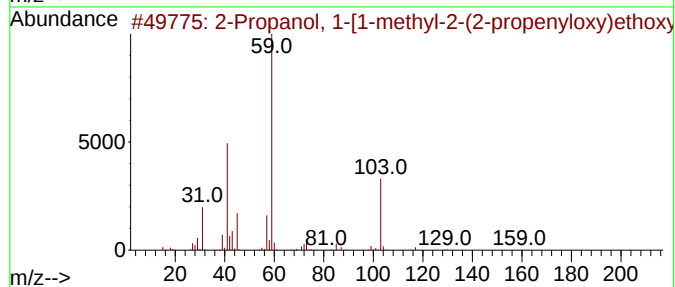
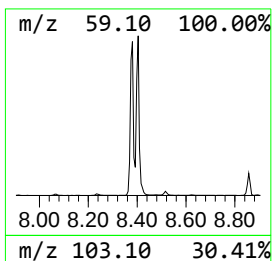
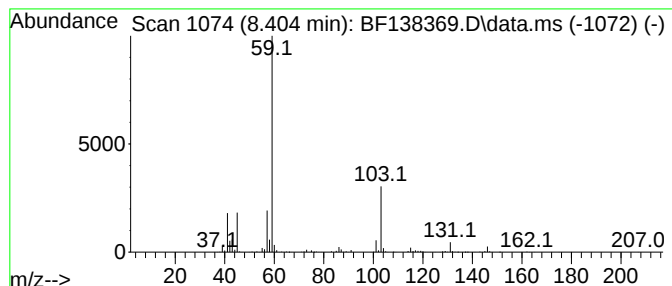
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.404	11.30 ng	982958	Naphthalene-d8	8.163

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		Methane, diethoxy-	104	C5H12O2	000462-95-3	72
3		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
4		2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	72
5		Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

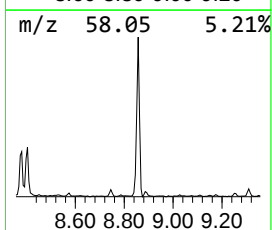
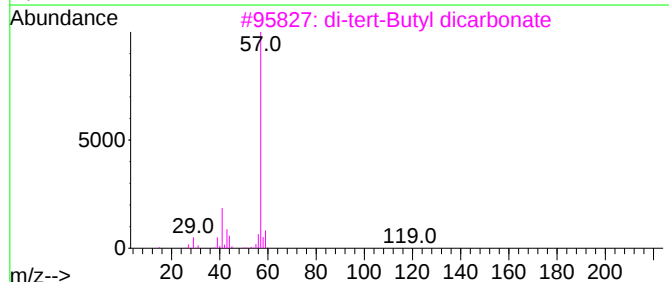
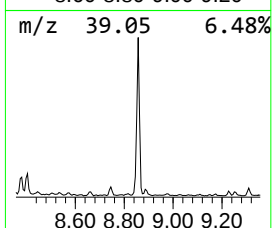
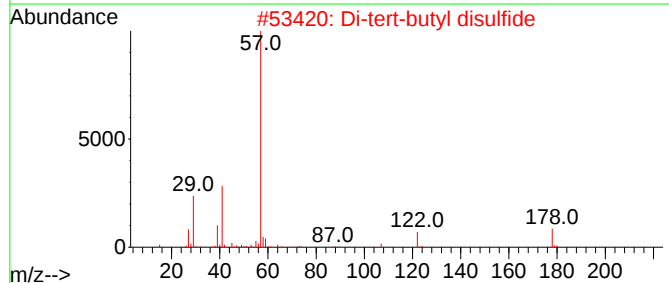
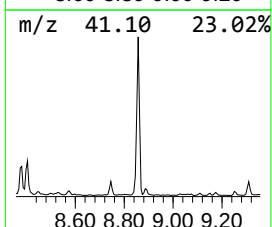
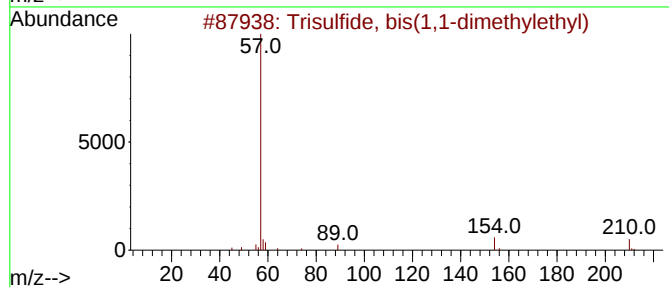
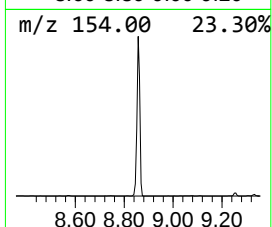
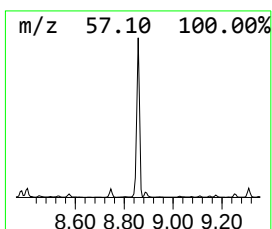
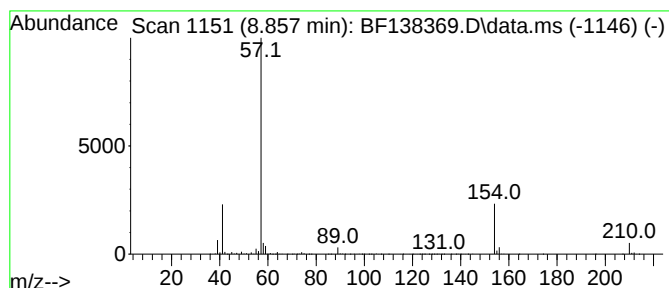
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Trisulfide, bis(1,1-dimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.857	35.61 ng	3097990	Naphthalene-d8	8.163

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	62
2		Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	35
3		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	12
4		di-tert-Butyl acetylenedicarboxy...	226	C12H18O4	066086-33-7	9
5		Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

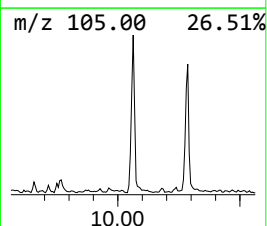
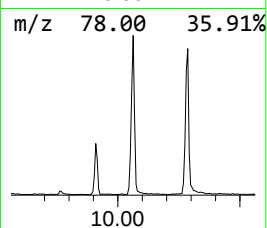
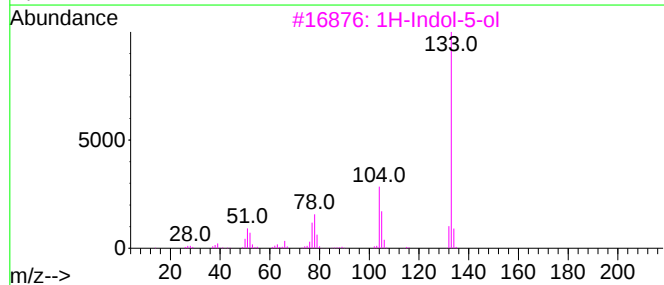
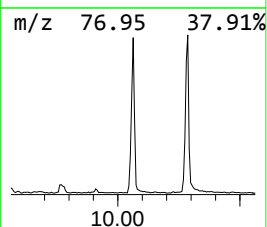
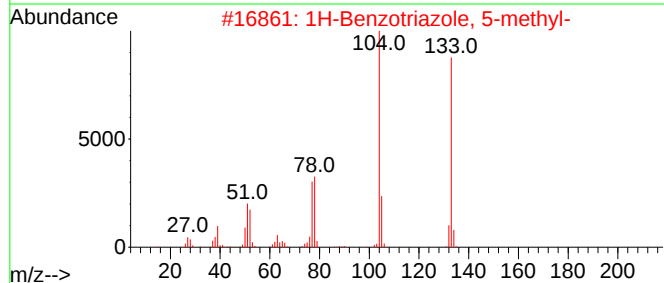
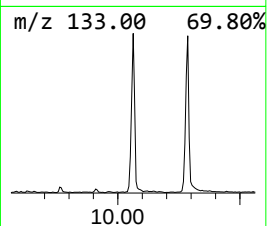
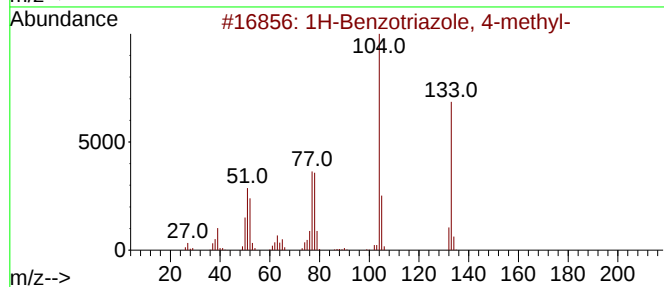
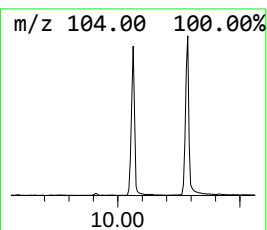
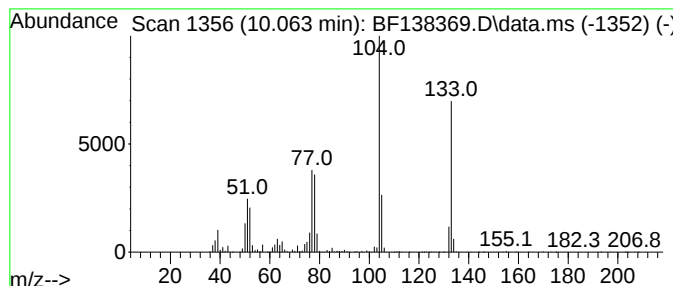
Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 1H-Benzotriazole, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.063	10.75 ng	946288	Acenaphthene-d10			9.910
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-		133	C7H7N3	029878-31-7	98
2	1H-Benzotriazole, 5-methyl-		133	C7H7N3	000136-85-6	97
3	1H-Indol-5-ol		133	C8H7NO	001953-54-4	87
4	2H-Indol-2-one, 1,3-dihydro-		133	C8H7NO	000059-48-3	76
5	Benzene, 1-azido-2-methyl-		133	C7H7N3	031656-92-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

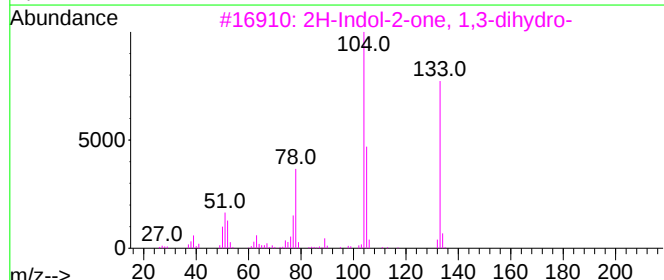
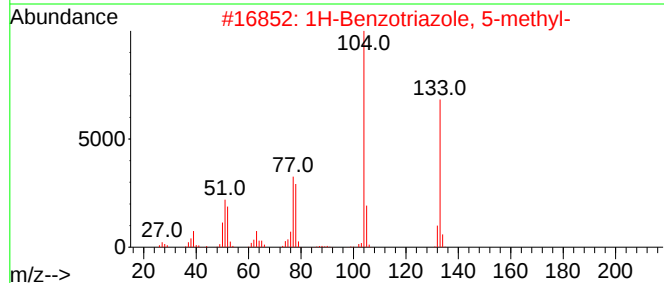
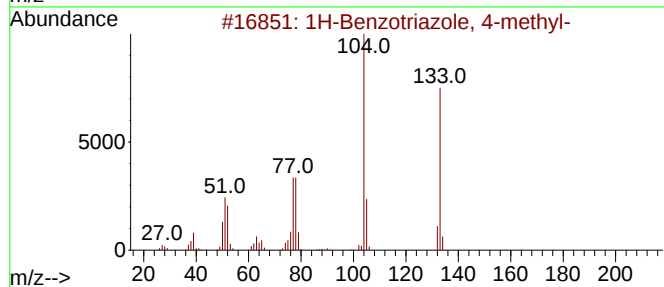
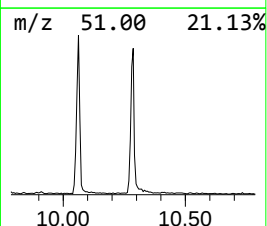
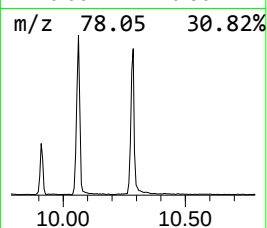
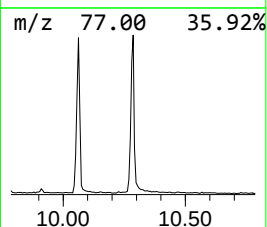
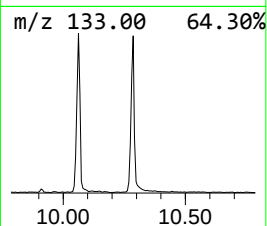
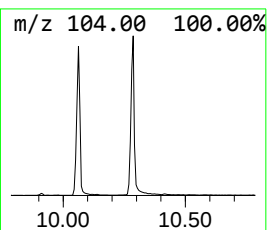
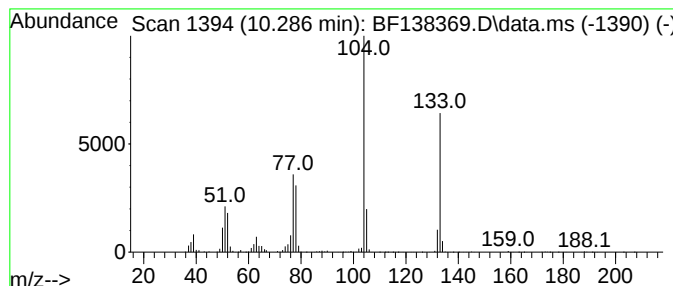
Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 1H-Benzotriazole, 5-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.286	9.18 ng	808056	Acenaphthene-d10			9.910
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-		133	C7H7N3	029878-31-7	98
2	1H-Benzotriazole, 5-methyl-		133	C7H7N3	000136-85-6	97
3	2H-Indol-2-one, 1,3-dihydro-		133	C8H7NO	000059-48-3	74
4	Phenol, 4-bromo-2-[(1H-indazol-7-...		317	C14H12BrN3O	1000350-54-6	52
5	N-Ethylbenzimidoyl bromide		211	C9H10BrN	041182-87-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

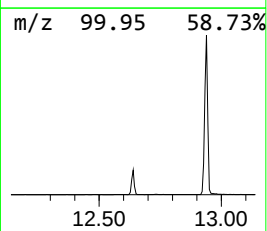
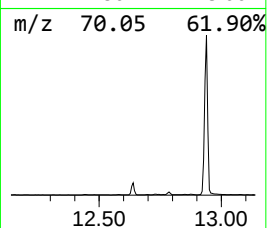
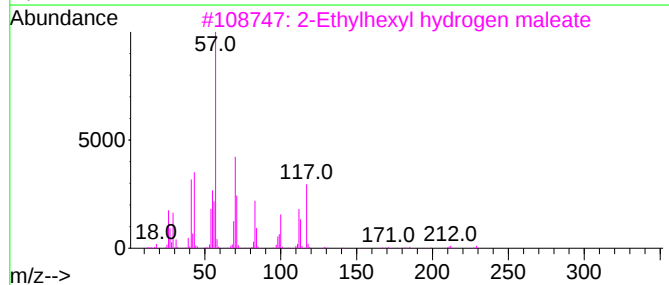
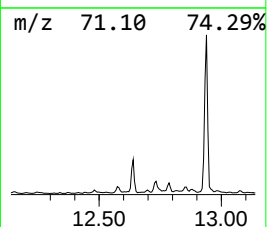
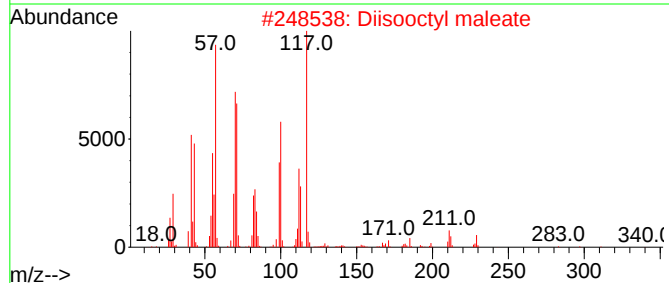
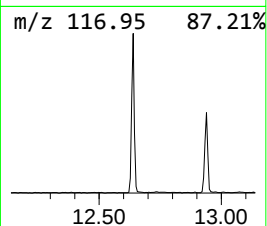
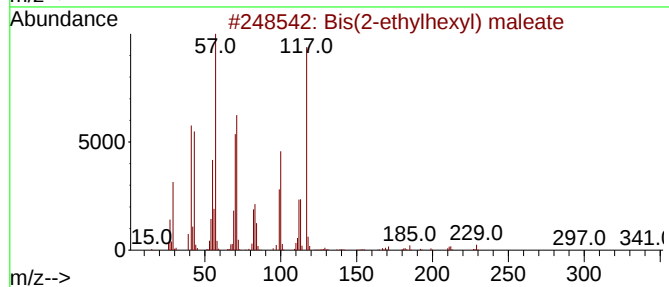
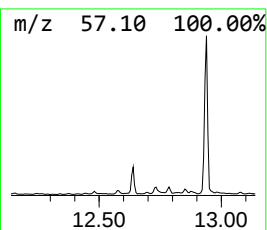
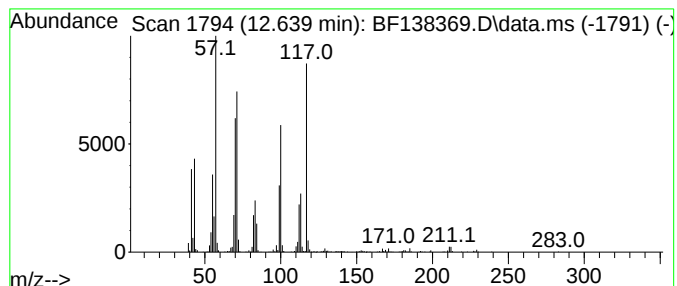
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Bis(2-ethylhexyl) maleate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	7.50 ng	554342	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	90
2			Diisooctyl maleate	340	C20H36O4	001330-76-3	49
3			2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	45
4			Carbonic acid, bis(2-ethylhexyl)...	286	C17H34O3	014858-73-2	43
5			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

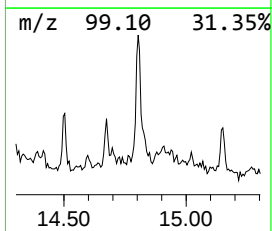
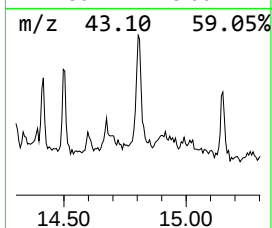
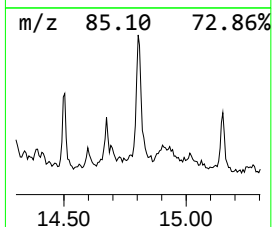
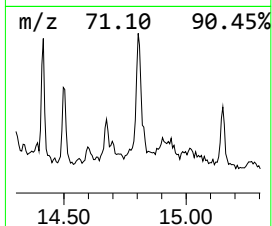
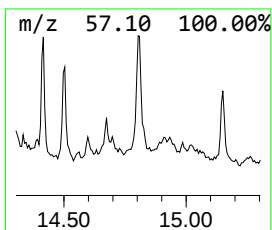
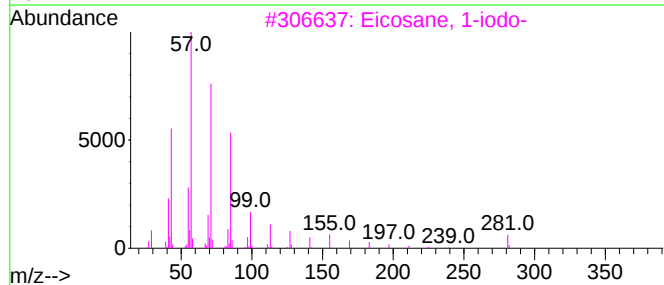
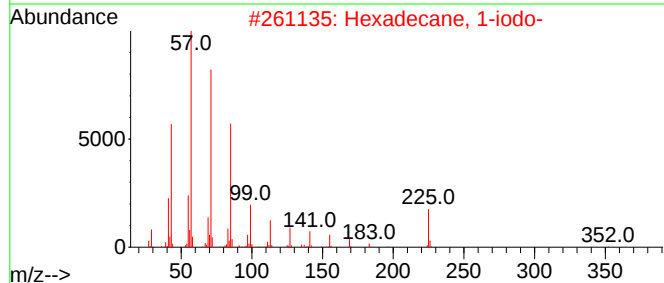
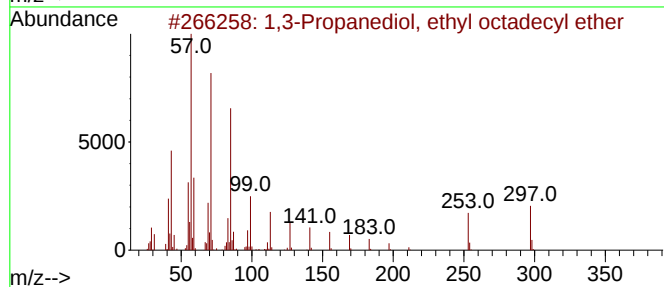
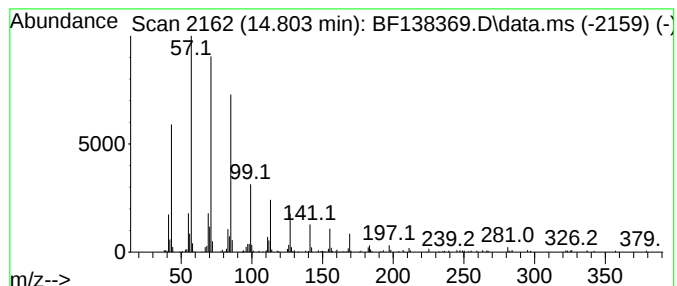
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 1,3-Propanediol, ethyl octa... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	4.93 ng	263277	Perylene-d12	15.503

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Propanediol, ethyl octadecyl...	356	C23H48O2	1000406-35-4	91
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90
3		Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90
4		Pentacosane	352	C25H52	000629-99-2	86
5		Docosane, 1-iodo-	436	C22H45I	1000406-31-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138369.D
Acq On : 27 Jun 2024 16:37
Operator : CG\JU
Sample : P3049-01 10X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.140	4.8	ng	366004	1	6.880	1508540	20.0
unknown2.492	2.492	6.3	ng	477868	1	6.880	1508540	20.0
Benzene, 1-ethy...	6.404	7.8	ng	584656	1	6.880	1508540	20.0
Decane	6.710	15.8	ng	1187830	1	6.880	1508540	20.0
Benzene, 1-ethy...	6.933	6.3	ng	477163	1	6.880	1508540	20.0
Benzene, 1-meth...	7.151	5.5	ng	414208	1	6.880	1508540	20.0
Benzene, 1,4-di...	7.198	6.0	ng	453292	1	6.880	1508540	20.0
Benzene, 1-meth...	7.269	5.9	ng	445674	1	6.880	1508540	20.0
unknown7.527	7.527	6.3	ng	547037	2	8.163	1740000	20.0
Hexanoic acid, ...	7.657	73.2	ng	6368980	2	8.163	1740000	20.0
Di-tert-butyl d...	7.704	7.0	ng	606384	2	8.163	1740000	20.0
1H-Indene, 2,3-...	7.898	7.0	ng	609867	2	8.163	1740000	20.0
2-Propanol, 1,1...	8.380	10.6	ng	925320	2	8.163	1740000	20.0
2-Propanol, 1-[...	8.404	11.3	ng	982958	2	8.163	1740000	20.0
Trisulfide, bis...	8.857	35.6	ng	3097990	2	8.163	1740000	20.0
1H-Benzotriazol...	10.063	10.8	ng	946288	3	9.910	1760770	20.0
1H-Benzotriazol...	10.286	9.2	ng	808056	3	9.910	1760770	20.0
Bis(2-ethylhexy...	12.639	7.5	ng	554342	4	11.398	1478560	20.0
1,3-Propanediol...	14.804	4.9	ng	263277	6	15.503	1067990	20.0