

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
 Data File : BF124977.D
 Acq On : 7 Aug 2021 16:46
 Operator : JU/CG
 Sample : M3297-05
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 121

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-BF080421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124977.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.446	567	571	574	rBV	42162	41108	4.11%	0.666%
2	5.769	621	626	627	rBV2	20520	33521	3.35%	0.543%
3	5.822	629	635	637	rVB	39559	72077	7.20%	1.167%
4	5.934	643	654	655	rBV3	16750	37824	3.78%	0.612%
5	6.310	712	718	719	rVV2	7069	11019	1.10%	0.178%
6	6.381	719	730	733	rVB3	16183	46559	4.65%	0.754%
7	6.481	741	747	751	rBV2	99391	132486	13.24%	2.145%
8	6.592	751	766	767	rBV2	15262	41193	4.12%	0.667%
9	6.645	767	775	776	rBV	13241	22322	2.23%	0.361%
10	6.704	783	785	787	rVB	40458	28757	2.87%	0.466%
11	6.828	803	806	809	rBV	47460	34379	3.43%	0.557%
12	6.875	809	814	817	rVV3	8672	13270	1.33%	0.215%
13	6.916	817	821	827	rVV4	12062	19102	1.91%	0.309%
14	6.975	827	831	833	rVV2	9980	14006	1.40%	0.227%
15	7.051	836	844	849	rVB3	17173	34024	3.40%	0.551%
16	7.128	849	857	859	rBV2	13468	21637	2.16%	0.350%
17	7.240	873	876	879	rBV3	15961	15902	1.59%	0.257%
18	7.322	879	890	893	rVV5	17285	56726	5.67%	0.918%
19	7.363	893	897	898	rVV3	11429	13195	1.32%	0.214%
20	7.392	898	902	905	rVB	82692	73258	7.32%	1.186%
21	7.581	923	934	936	rBV2	50291	94497	9.44%	1.530%
22	7.775	945	967	972	rVB3	171454	1000934	100.00%	16.205%
23	7.822	972	975	978	rVB2	31821	28671	2.86%	0.464%
24	7.863	980	982	984	rVB	24071	16593	1.66%	0.269%
25	7.957	991	998	999	rBV2	16901	25882	2.59%	0.419%
26	8.010	999	1007	1009	rVB2	30149	56240	5.62%	0.911%
27	8.081	1016	1019	1022	rBV2	21378	22599	2.26%	0.366%
28	8.110	1022	1024	1027	rVB	55943	42487	4.24%	0.688%
29	8.145	1027	1030	1032	rVB	19891	16893	1.69%	0.273%
30	8.204	1038	1040	1044	rBV3	18893	23401	2.34%	0.379%
31	8.239	1044	1046	1048	rVB2	16764	12859	1.28%	0.208%
32	8.304	1050	1057	1062	rBV3	41657	107104	10.70%	1.734%
33	8.345	1062	1064	1069	rVB3	9972	11295	1.13%	0.183%
34	8.398	1069	1073	1075	rBV3	11494	11656	1.16%	0.189%
35	8.469	1075	1085	1087	rBV	76627	144167	14.40%	2.334%
36	8.569	1087	1102	1104	rVV	169637	616497	61.59%	9.981%

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Sampling : 1

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Max Peaks: 100

Stop Thrs : 0

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37	8.592	1104	1106	1107	rVV2	14516	11395	1.14%	0.184%
38	8.616	1107	1110	1113	rVV3	30809	29664	2.96%	0.480%
39	8.657	1113	1117	1118	rVV3	13203	16371	1.64%	0.265%
40	8.675	1118	1120	1122	rVB	38789	25919	2.59%	0.420%
41	8.722	1126	1128	1132	rVB3	17447	19520	1.95%	0.316%
42	8.786	1136	1139	1141	rBV	20990	18083	1.81%	0.293%
43	8.816	1141	1144	1149	rVB2	55739	63346	6.33%	1.026%
44	8.869	1149	1153	1157	rBV2	43779	71650	7.16%	1.160%
45	8.916	1157	1161	1163	rBV	42009	34429	3.44%	0.557%
46	9.057	1167	1185	1191	rBV	169440	576436	57.59%	9.332%
47	9.145	1198	1200	1203	rVB3	24045	18559	1.85%	0.300%
48	9.186	1203	1207	1211	rBV	189824	158713	15.86%	2.570%
49	9.228	1211	1214	1216	rBV3	17211	14745	1.47%	0.239%
50	9.316	1227	1229	1232	rBV	25988	25630	2.56%	0.415%
51	9.345	1232	1234	1237	rVV2	53047	42213	4.22%	0.683%
52	9.386	1237	1241	1245	rVV	23125	32241	3.22%	0.522%
53	9.463	1251	1254	1258	rBV2	22200	25454	2.54%	0.412%
54	9.763	1299	1305	1308	rBV3	19062	27593	2.76%	0.447%
55	9.845	1308	1319	1321	rVV2	141277	272534	27.23%	4.412%
56	9.863	1321	1322	1325	rVV	149780	103419	10.33%	1.674%
57	9.892	1325	1327	1329	rVV3	12358	12133	1.21%	0.196%
58	9.916	1329	1331	1334	rVV3	20277	18952	1.89%	0.307%
59	9.981	1338	1342	1343	rBV3	9282	10883	1.09%	0.176%
60	10.051	1351	1354	1359	rVB6	10616	19326	1.93%	0.313%
61	10.110	1359	1364	1366	rBV4	12242	14582	1.46%	0.236%
62	10.304	1396	1397	1400	rVV2	13861	11399	1.14%	0.185%
63	10.439	1417	1420	1423	rBV3	22252	19574	1.96%	0.317%
64	10.622	1448	1451	1454	rVB4	10827	12688	1.27%	0.205%
65	10.657	1454	1457	1461	rBV	64830	54625	5.46%	0.884%
66	10.733	1468	1470	1477	rBV8	5626	11055	1.10%	0.179%
67	10.792	1477	1480	1485	rVV6	16810	18528	1.85%	0.300%
68	11.351	1572	1575	1578	rBV	64362	57558	5.75%	0.932%
69	11.904	1660	1669	1678	rBV	141648	193492	19.33%	3.133%
70	12.363	1743	1747	1748	rBV4	8625	11736	1.17%	0.190%
71	12.598	1782	1787	1790	rBV4	26397	42766	4.27%	0.692%
72	12.698	1793	1804	1808	rVB	277384	462598	46.22%	7.489%
73	12.839	1823	1828	1837	rVB3	49577	99234	9.91%	1.607%
74	12.939	1841	1845	1848	rVB	141182	118035	11.79%	1.911%
75	13.080	1867	1869	1873	rVB4	9894	11014	1.10%	0.178%
76	13.263	1896	1900	1908	rVB7	19658	35466	3.54%	0.574%

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Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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77	13.392	1920	1922	1928	rVB7	11804	13530	1.35%	0.219%
78	13.916	2007	2011	2018	rVB2	32775	51620	5.16%	0.836%
79	13.998	2022	2025	2028	rVV	47804	43911	4.39%	0.711%
80	14.445	2096	2101	2107	rVB2	35176	52825	5.28%	0.855%
81	14.833	2163	2167	2174	rVB4	10344	18811	1.88%	0.305%
82	14.939	2181	2185	2191	rBV2	28826	44126	4.41%	0.714%
83	15.457	2268	2273	2276	rBV	28844	34420	3.44%	0.557%
84	15.498	2276	2280	2288	rVB2	18584	31511	3.15%	0.510%
85	16.133	2378	2388	2396	rVB3	11263	24272	2.42%	0.393%
86	16.533	2448	2456	2462	rBV5	4910	11023	1.10%	0.178%
87	16.868	2506	2513	2518	rBV4	5747	11157	1.11%	0.181%
88	17.727	2651	2659	2664	rBV3	4305	11603	1.16%	0.188%
89	18.721	2821	2828	2833	rBV2	4098	10179	1.02%	0.165%

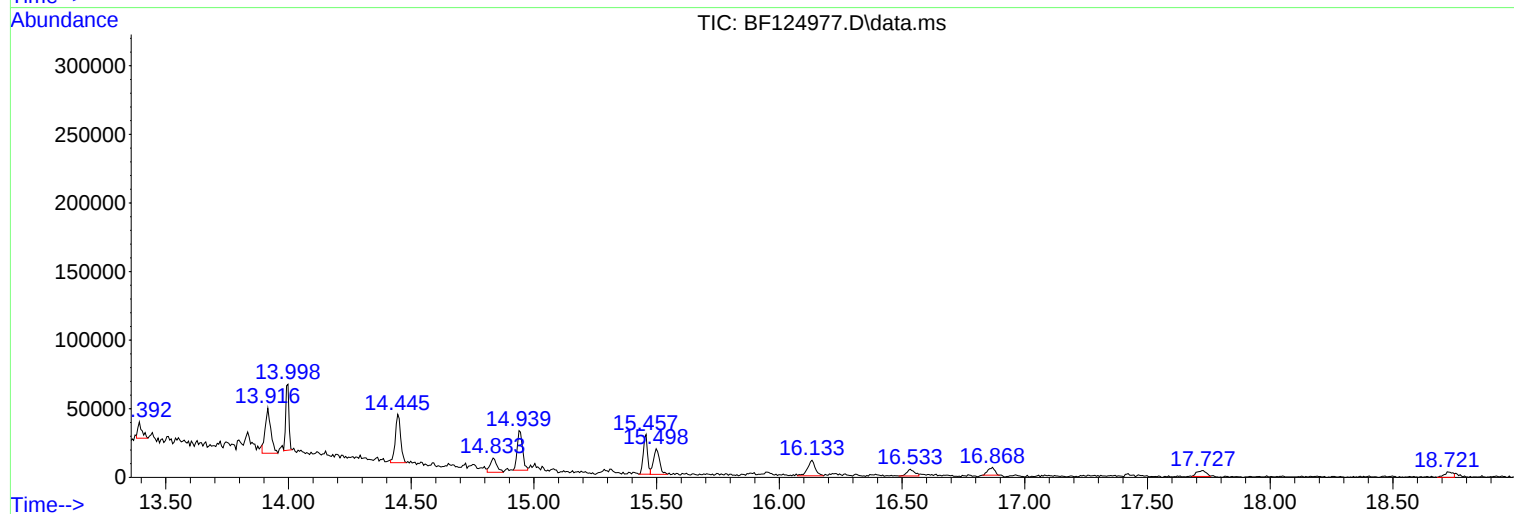
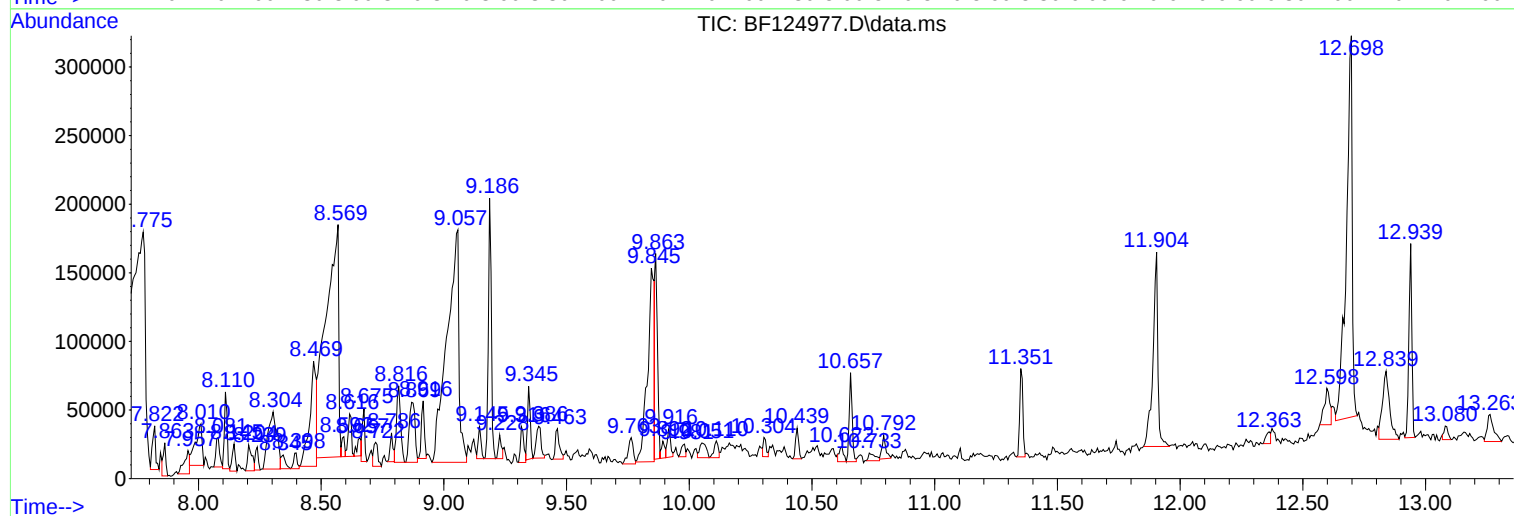
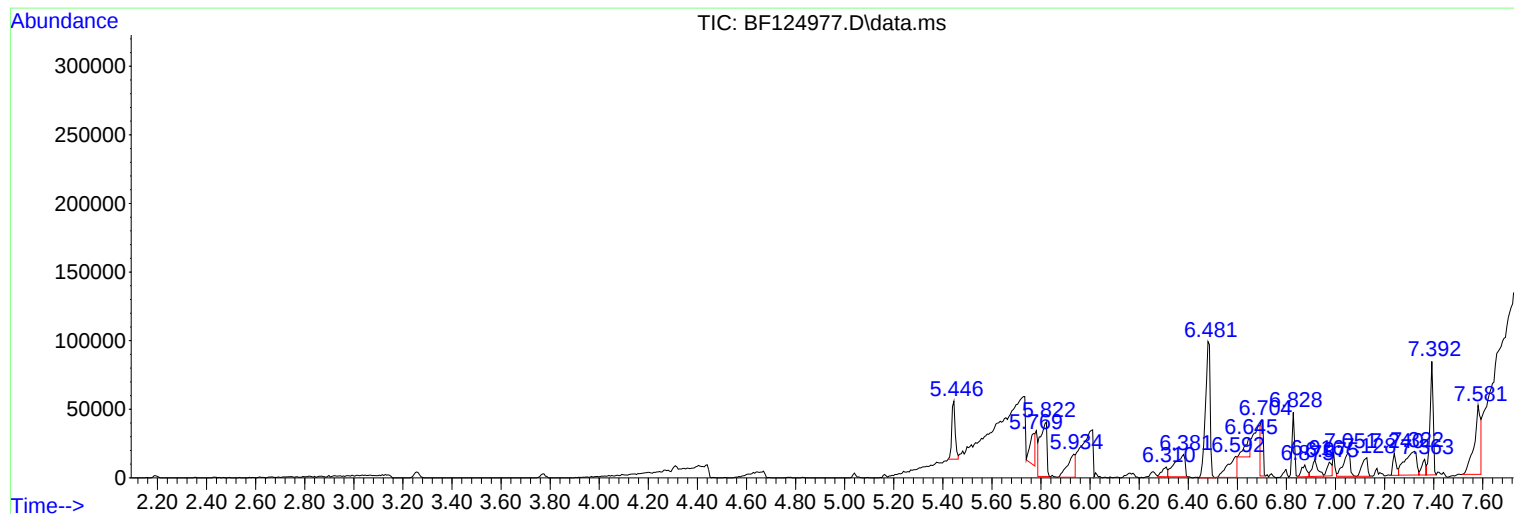
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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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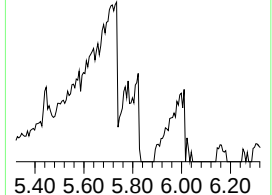
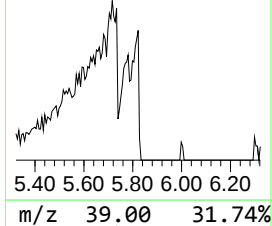
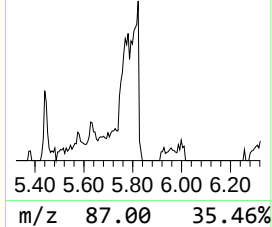
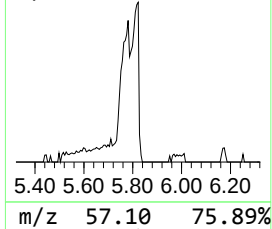
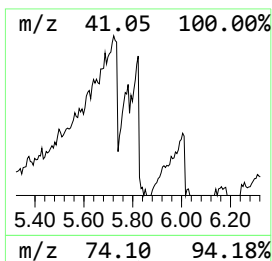
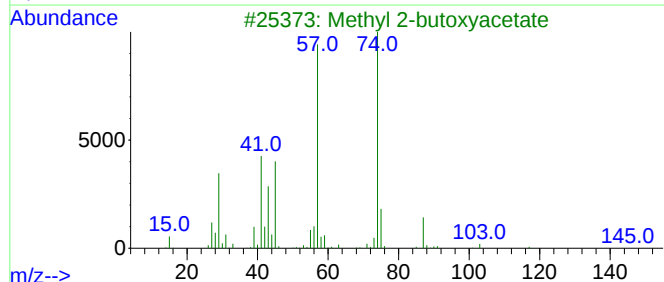
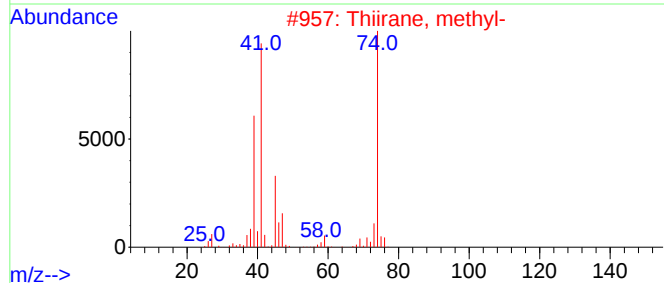
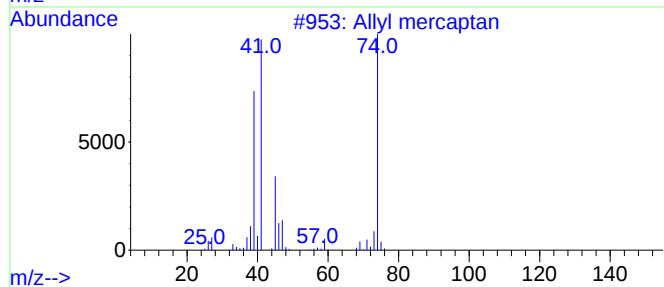
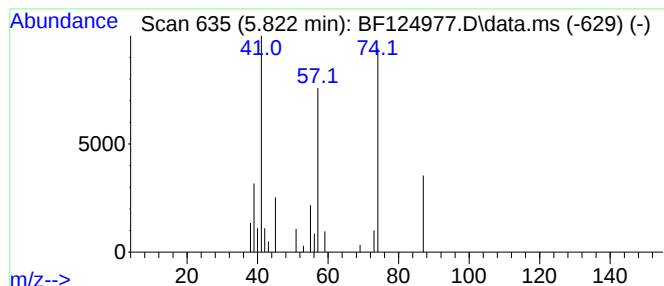
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Allyl mercaptan Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.822	41.93 ng	72077	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Allyl mercaptan	74	C3H6S	000870-23-5	53
2			Thiirane, methyl-	74	C3H6S	001072-43-1	38
3			Methyl 2-butoxyacetate	146	C7H14O3	1000366-88-4	36
4			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	25
5			1-Pentanamine	87	C5H13N	000110-58-7	9



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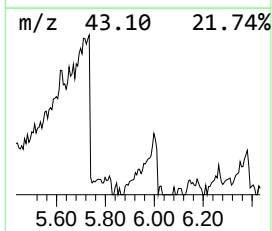
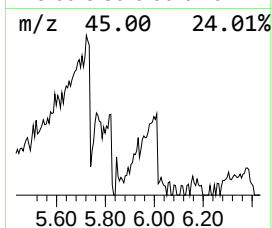
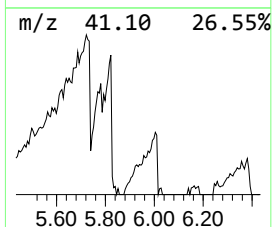
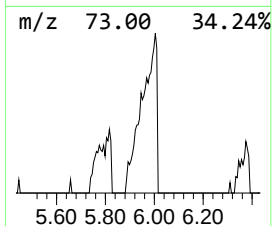
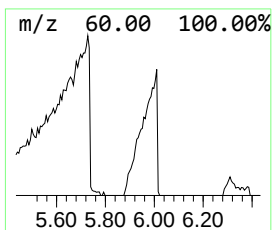
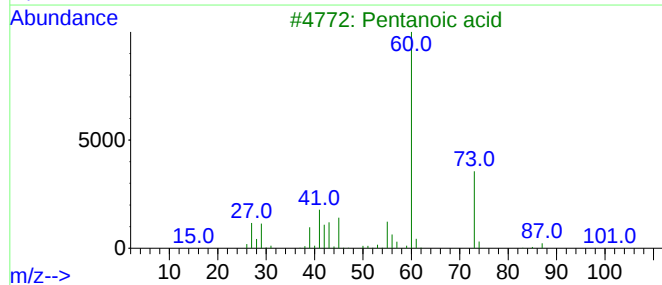
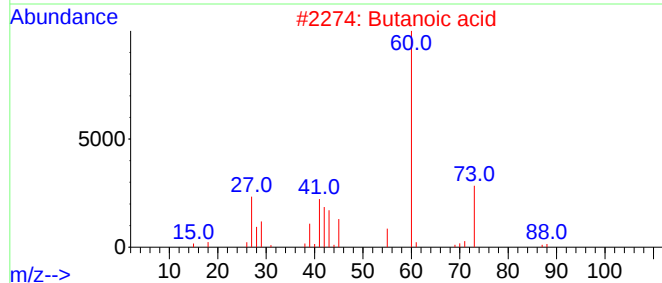
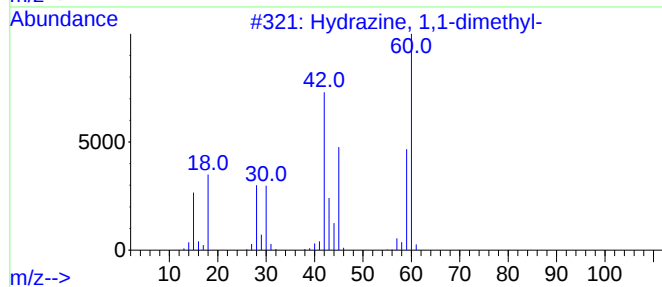
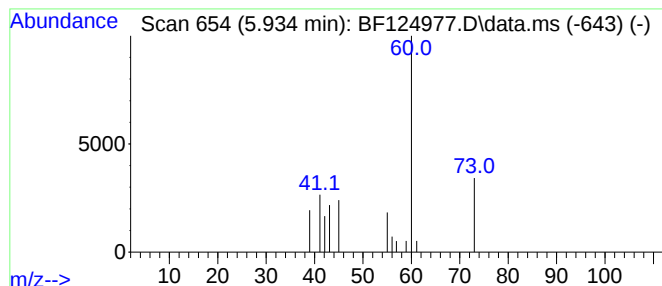
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.934 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.934	22.00 ng	37824	1,4-Dichlorobenzene-d4	6.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
2		Butanoic acid	88	C4H8O2	000107-92-6	9
3		Pentanoic acid	102	C5H10O2	000109-52-4	9
4		Formic acid hydrazide	60	CH4N2O	000624-84-0	5
5		Isobutylamine	73	C4H11N	000078-81-9	5



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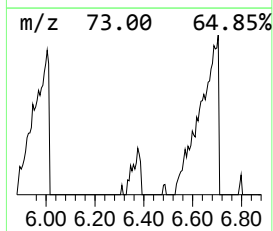
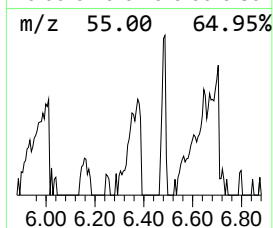
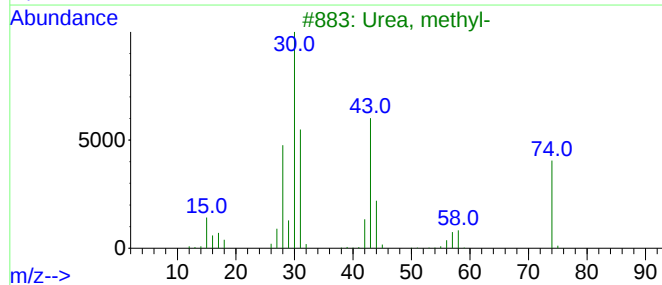
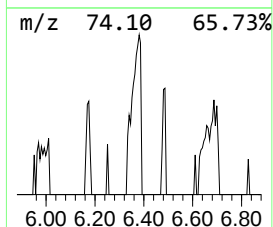
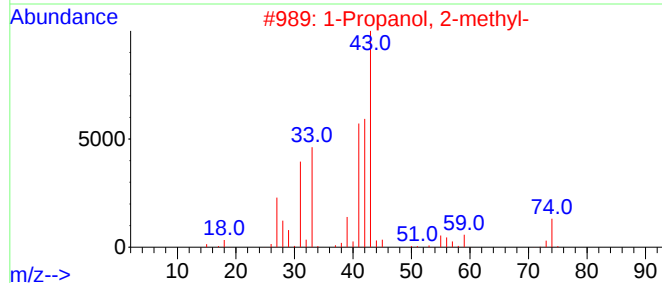
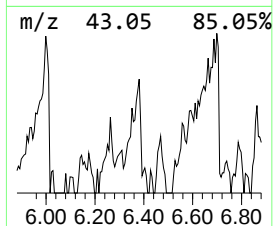
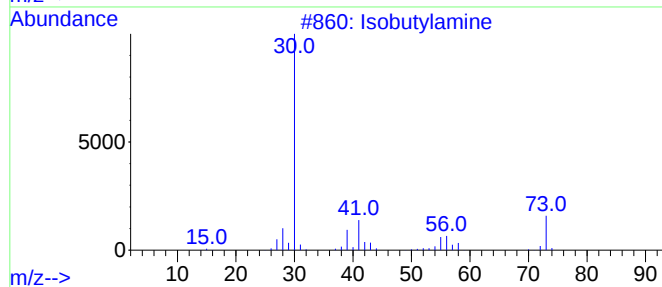
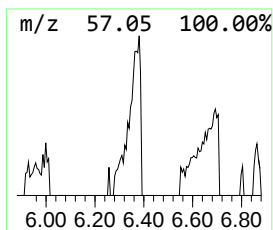
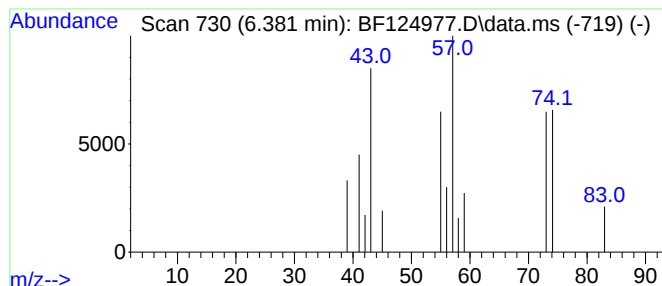
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.381 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.381	27.09 ng	46559	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutylamine	73	C4H11N	000078-81-9	9
2			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3			Urea, methyl-	74	C2H6N2O	000598-50-5	9
4			tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	9
5			1,5-Pentanediol	104	C5H12O2	000111-29-5	9



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ClientSampleId :
121

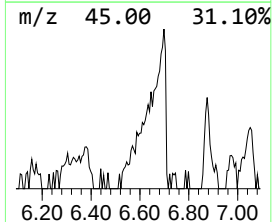
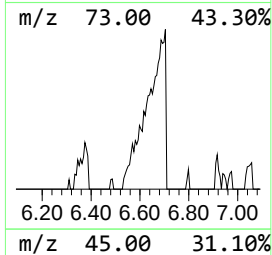
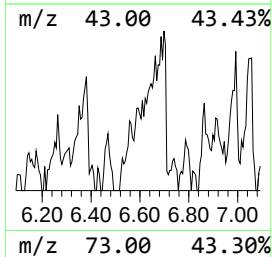
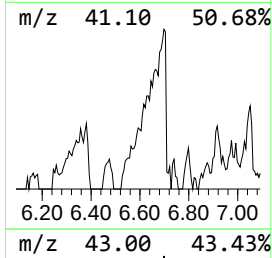
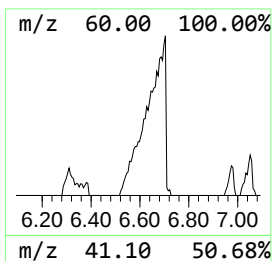
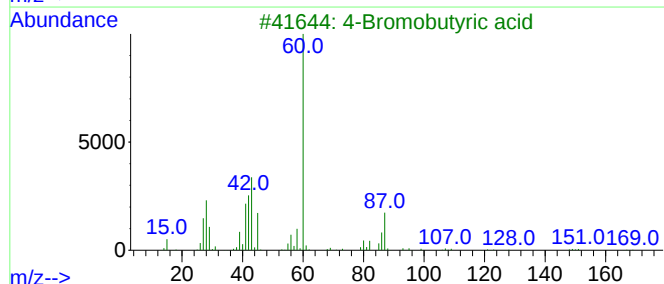
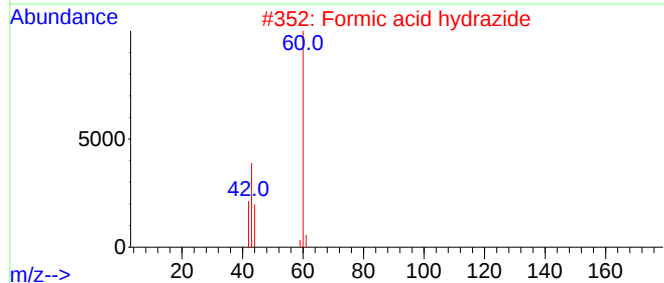
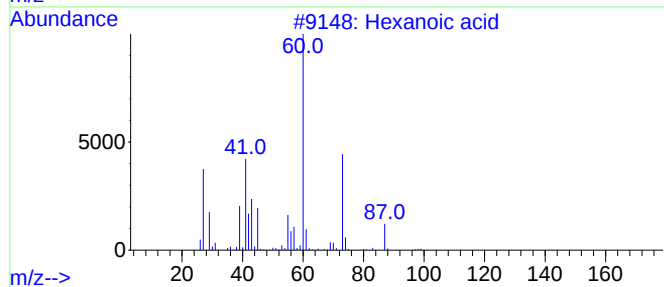
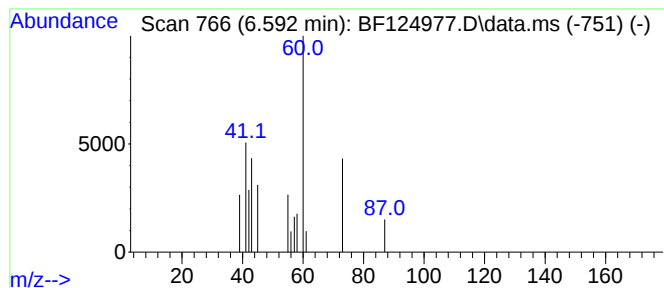
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.592	23.96 ng	41193	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid	116	C6H12O2	000142-62-1	72
2			Formic acid hydrazide	60	CH4N2O	000624-84-0	40
3			4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	38
4			Guanidine, methyl-	73	C2H7N3	000471-29-4	9
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124977.D
Acq On : 7 Aug 2021 16:46
Operator : JU/CG
Sample : M3297-05
Misc :
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Instrument :
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ClientSampled :
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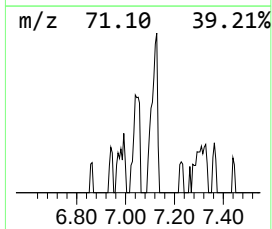
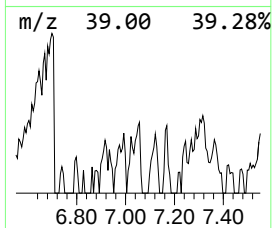
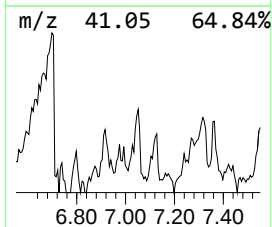
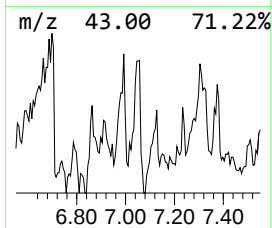
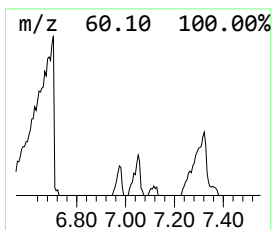
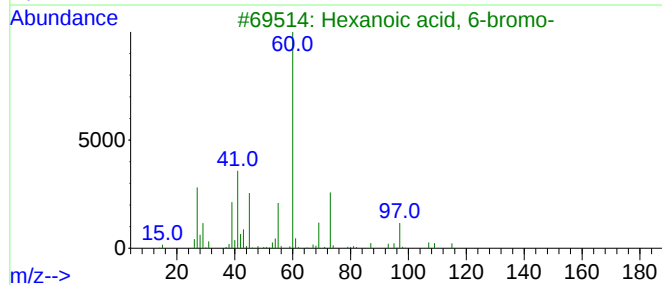
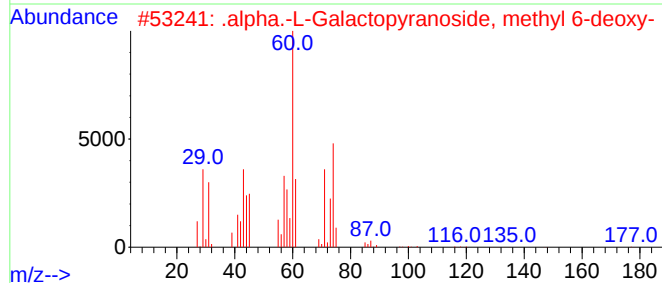
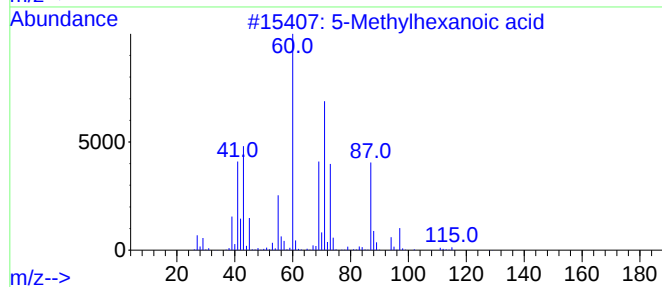
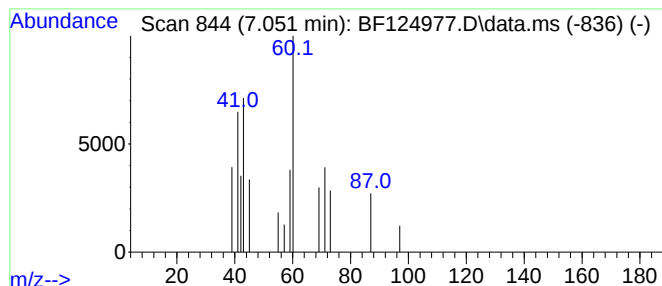
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 5-Methylhexanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.051	19.79 ng	34024	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Methylhexanoic acid	130	C7H14O2	000628-46-6	59
2			.alpha.-L-Galactopyranoside, met...	178	C7H14O5	014687-15-1	33
3			Hexanoic acid, 6-bromo-	194	C6H11BrO2	004224-70-8	32
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5			Pentanoic acid, 2-hydroxy-4-meth...	146	C7H14O3	040348-72-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124977.D
Acq On : 7 Aug 2021 16:46
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Sample : M3297-05
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Instrument :
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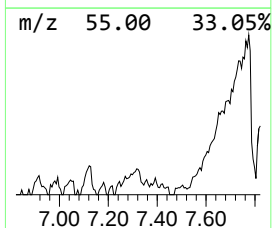
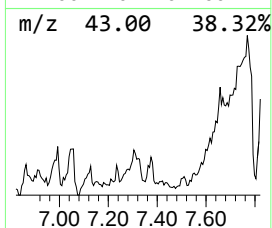
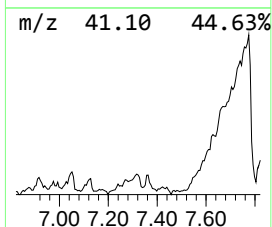
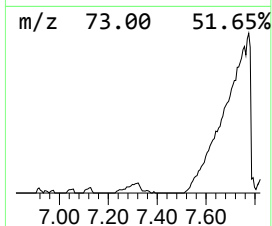
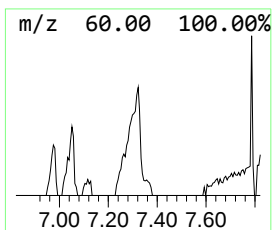
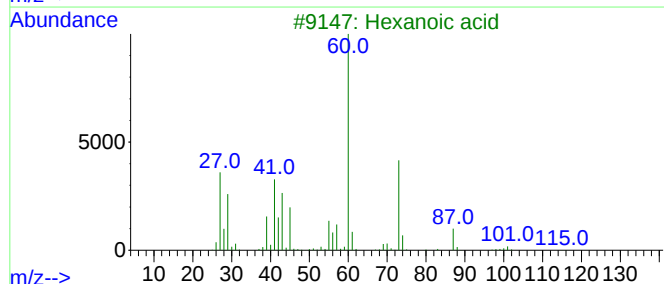
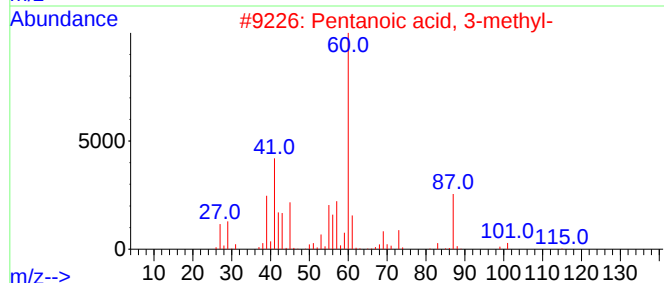
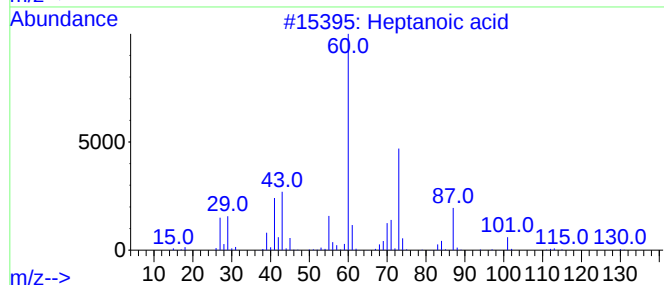
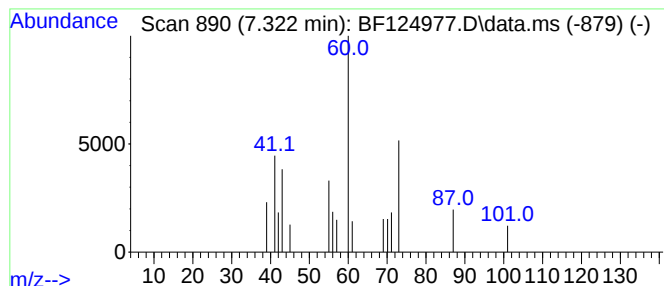
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.322	33.00 ng	56726	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanoic acid	130	C7H14O2	000111-14-8	72
2			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	59
3			Hexanoic acid	116	C6H12O2	000142-62-1	59
4			.beta.-Methyl xyloside	164	C6H12O5	007473-45-2	37
5			3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124977.D
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Instrument :
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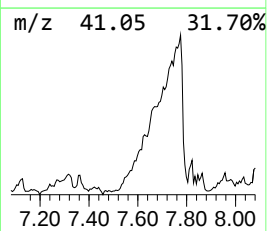
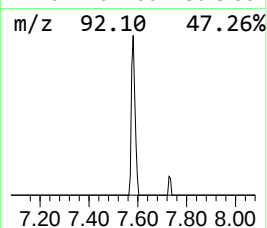
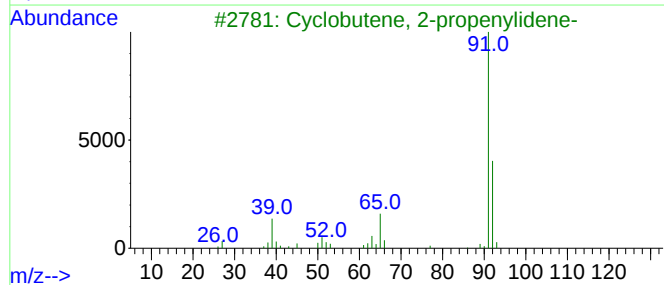
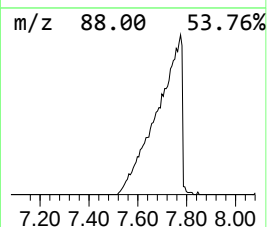
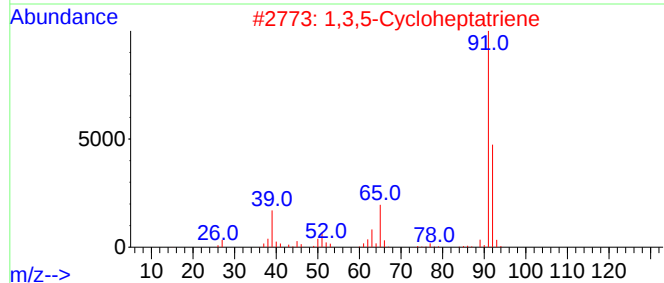
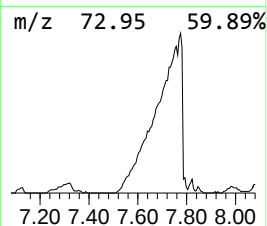
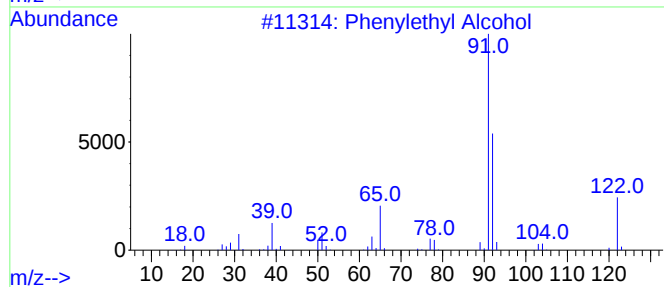
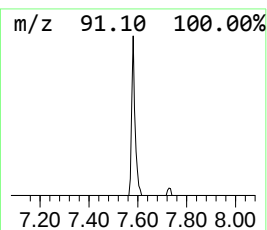
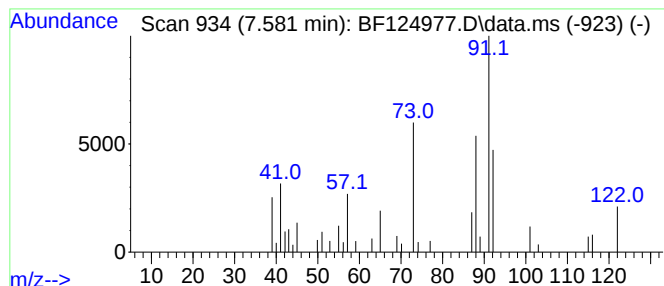
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown7.581 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.581	44.48 ng	94497	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenylethyl Alcohol	122	C8H10O	000060-12-8	46
2			1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	38
3			Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	35
4			Bicyclo[3.2.0]hepta-2,6-diene	92	C7H8	002422-86-8	35
5			Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	35



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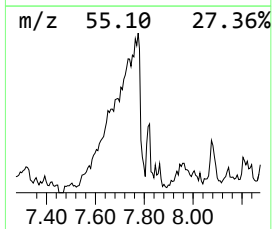
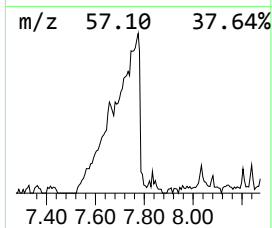
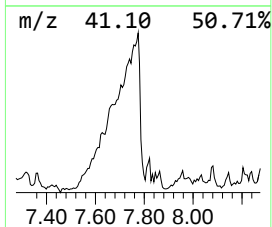
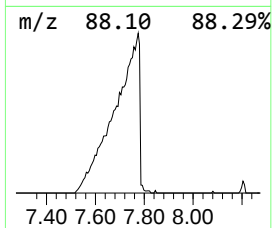
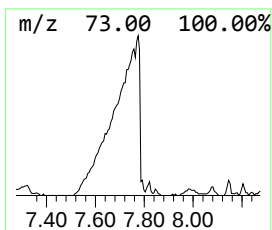
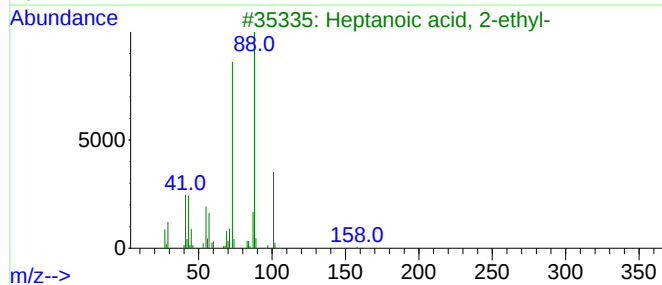
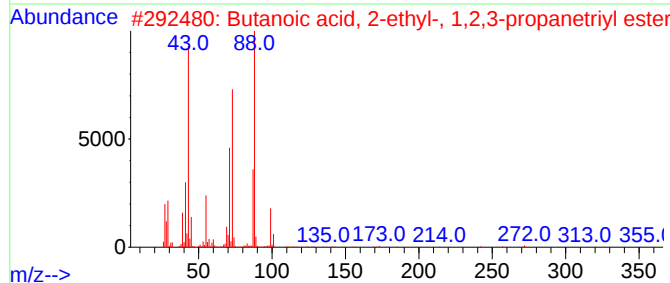
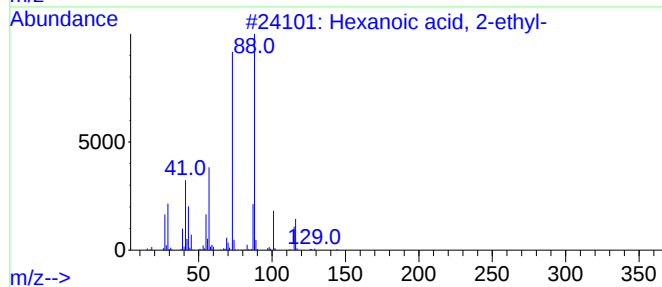
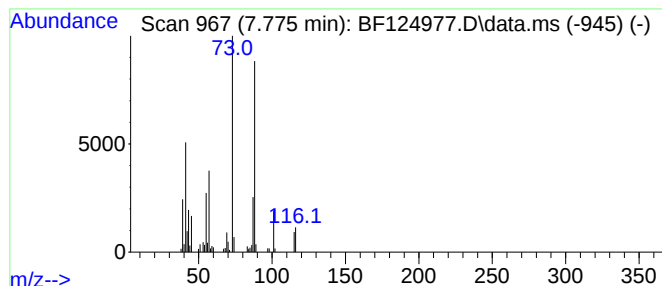
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.775	471.17 ng	1000930	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	80
2			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
4			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	45
5			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	42



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Data File : BF124977.D
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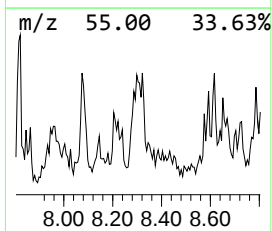
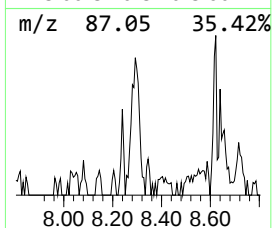
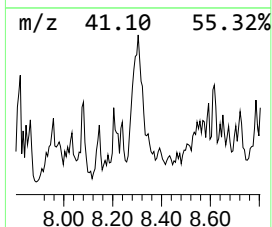
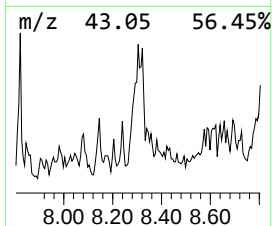
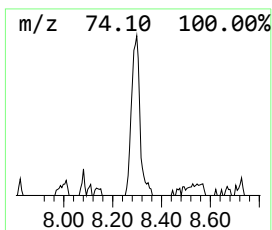
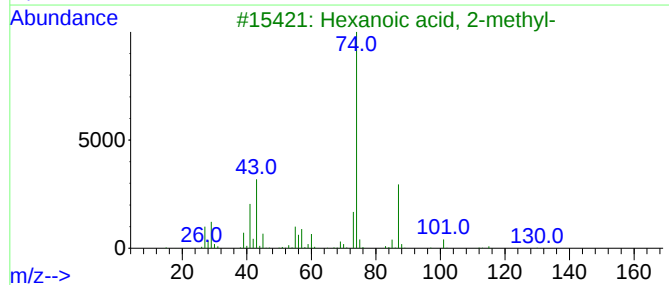
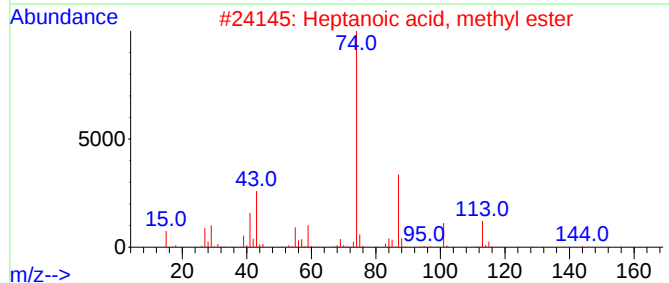
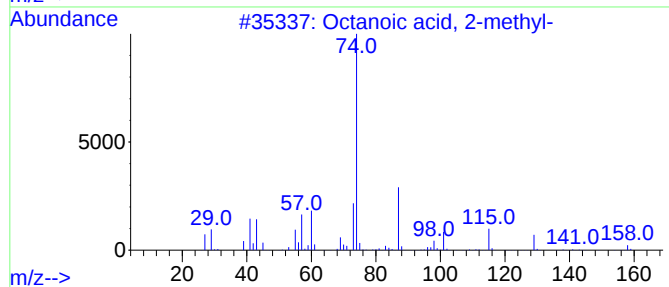
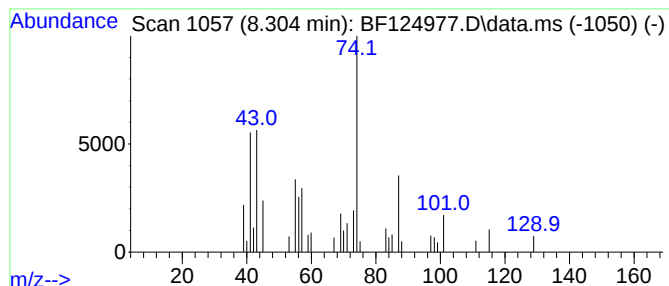
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octanoic acid, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.304	50.42 ng	107104	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	53
2			Heptanoic acid, methyl ester	144	C8H16O2	000106-73-0	43
3			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	42
4			Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	38
5			2-(Hexyloxy)acetic acid, methyl ...	174	C9H18O3	070038-38-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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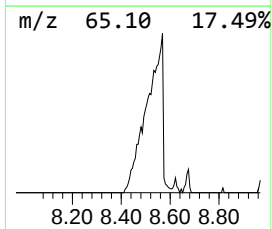
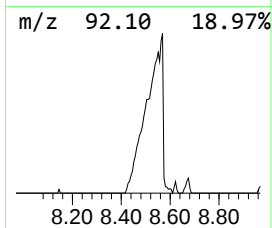
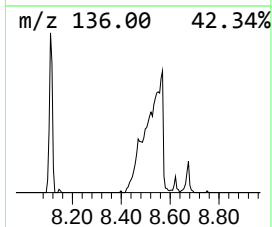
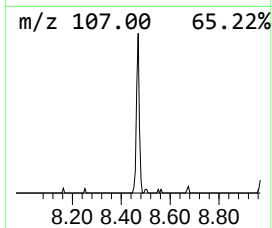
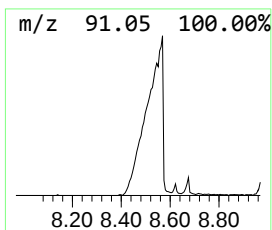
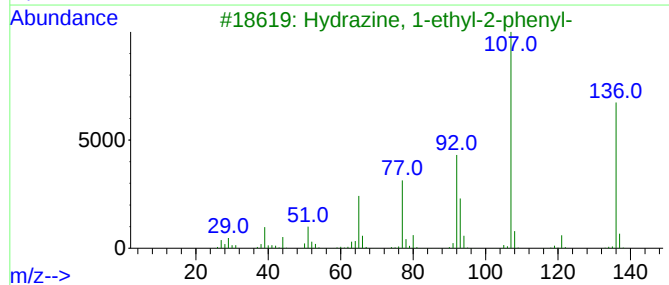
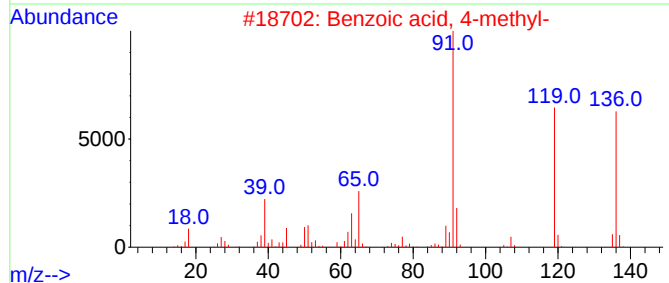
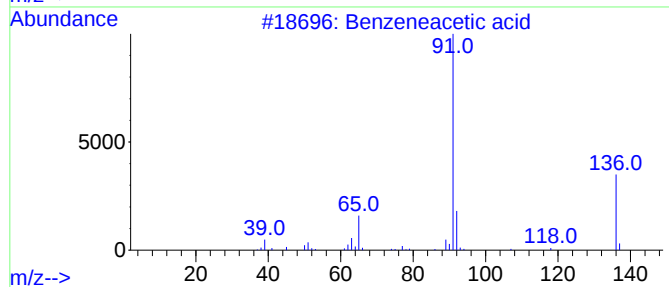
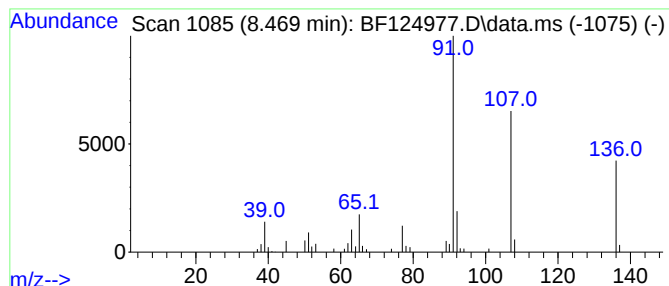
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzoic acid, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	67.86 ng	144167	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenecetic acid	136	C8H8O2	000103-82-2	64
2			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	53
3			Hydrazine, 1-ethyl-2-phenyl-	136	C8H12N2	000622-82-2	52
4			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	50
5			Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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Sample : M3297-05
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ClientSampleId :
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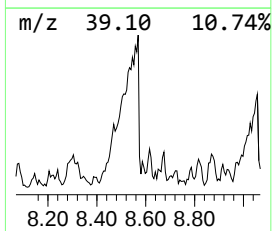
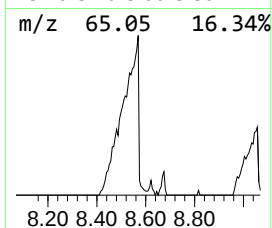
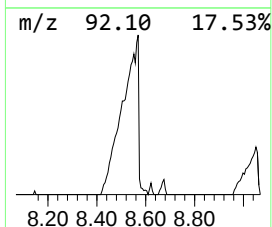
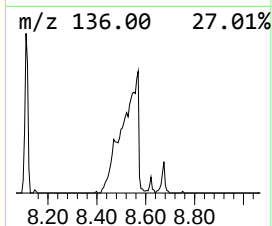
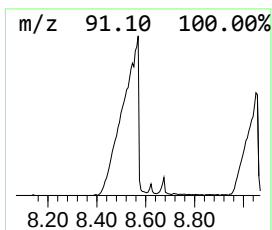
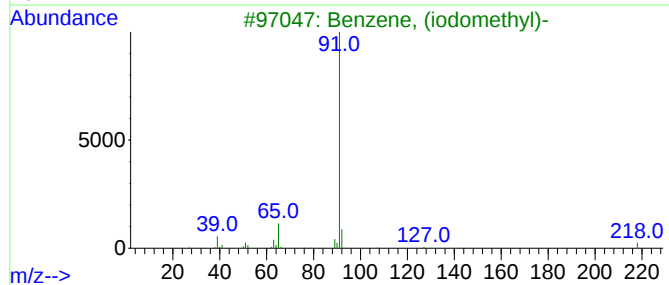
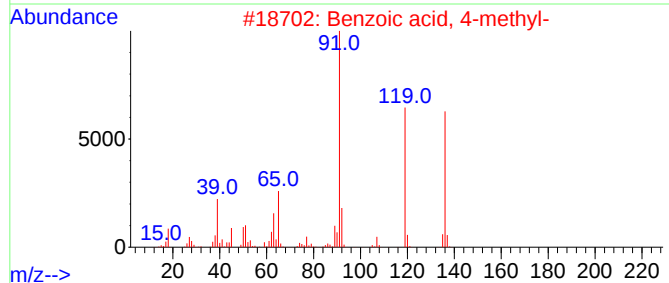
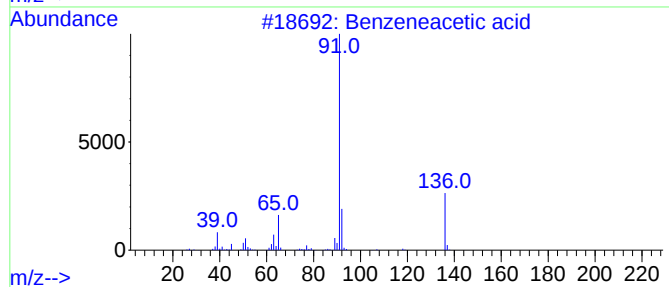
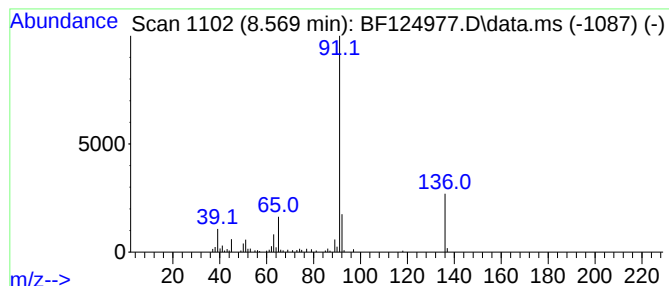
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzeneacetic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.569	290.20 ng	616497	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	93
2			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	52
3			Benzene, (iodomethyl)-	218	C7H7I	000620-05-3	50
4			12-Benzyl-4,9,15-trioxa-3,5,8,10...	325	C13H7N7O4	1394125-25-7	47
5			Benzyl 2-chloroethyl sulfone	218	C9H11ClO2S	066998-67-2	47



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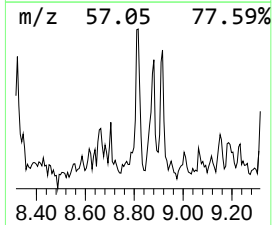
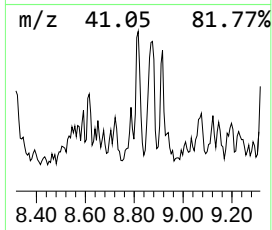
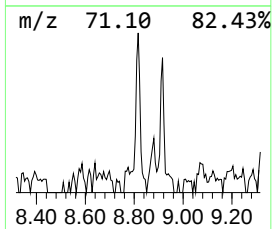
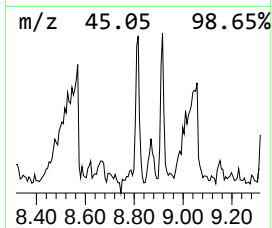
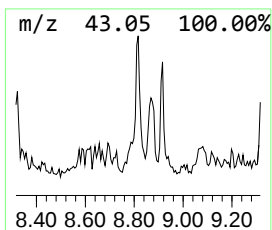
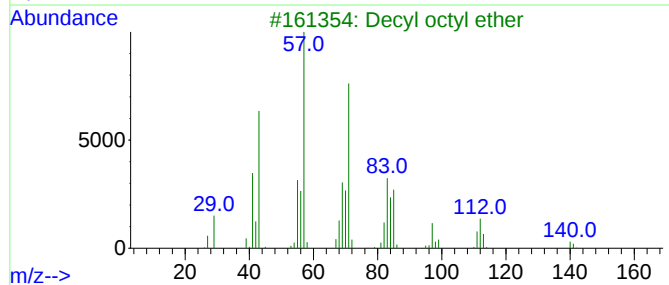
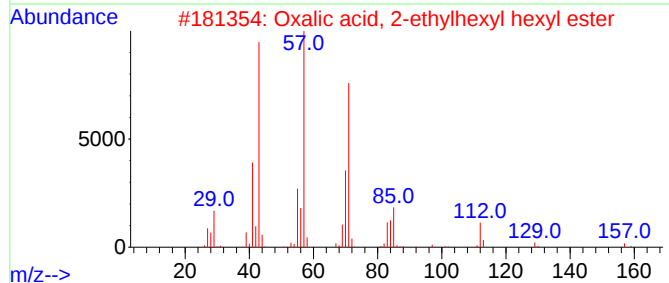
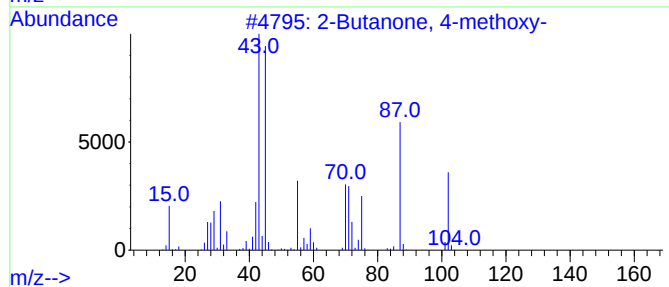
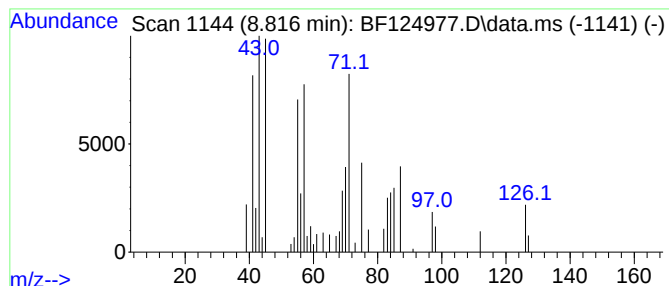
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown8.816 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.816	29.82 ng	63346	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 4-methoxy-			102	C5H10O2	006975-85-5	43
2	Oxalic acid, 2-ethylhexyl hexyl ...			286	C16H30O4	1000309-38-9	27
3	Decyl octyl ether			270	C18H38O	1000406-38-3	27
4	Undecane, 4-methyl-			170	C12H26	002980-69-0	27
5	Dodecane, 2,6,10-trimethyl-			212	C15H32	003891-98-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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Sample : M3297-05
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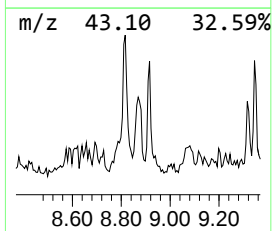
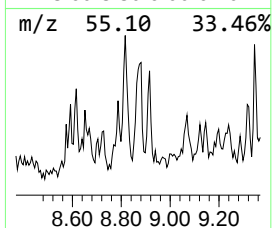
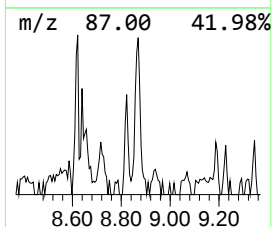
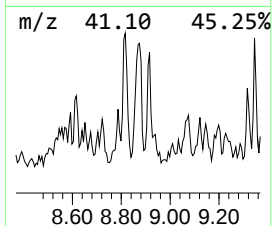
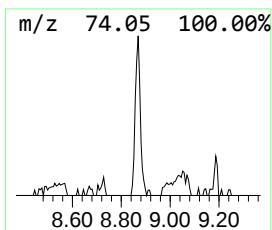
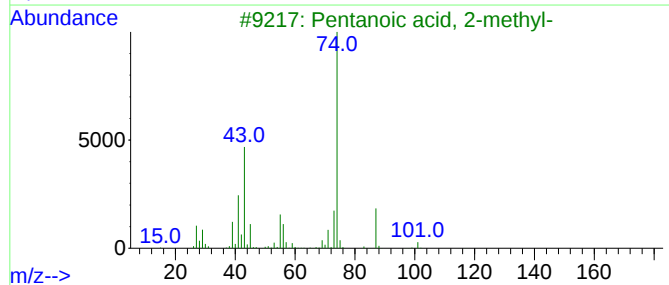
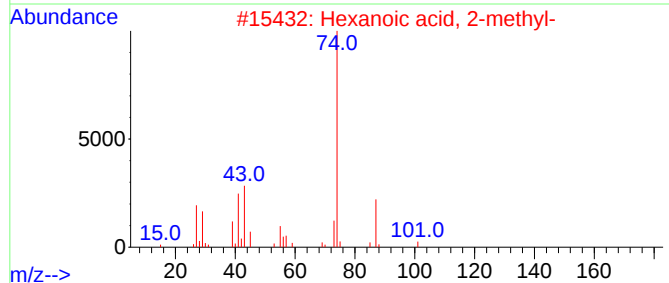
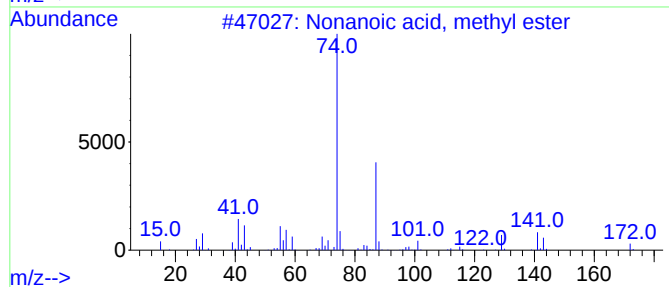
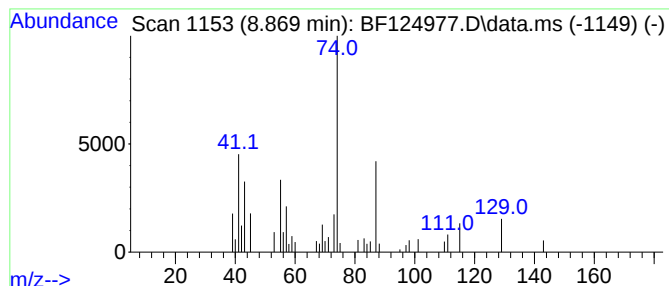
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Nonanoic acid, methyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.869	33.73 ng	71650	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	64
2			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	59
3			Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	59
4			Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	56
5			Decanoic acid, 2-methyl-	186	C11H22O2	024323-23-7	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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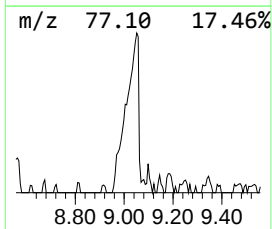
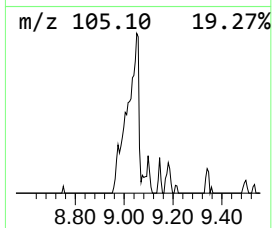
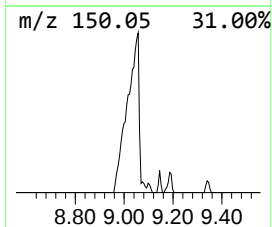
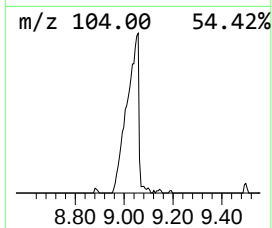
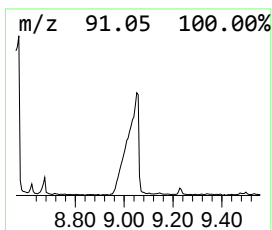
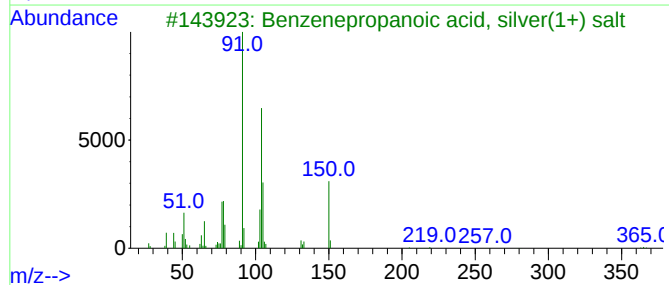
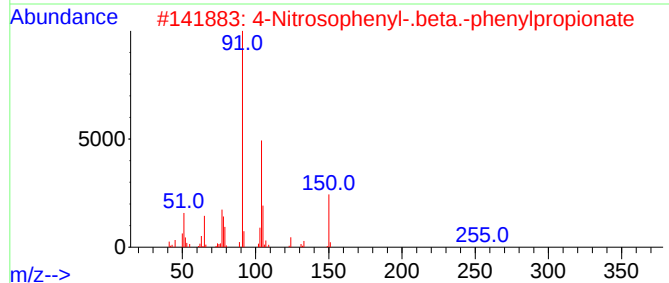
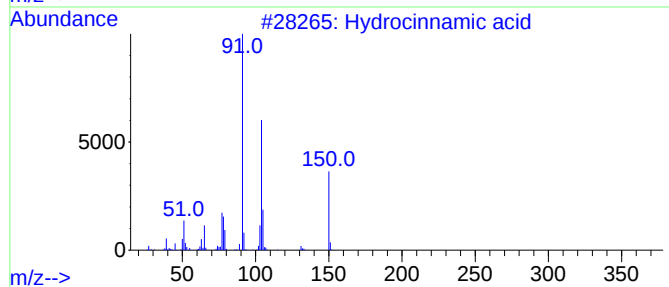
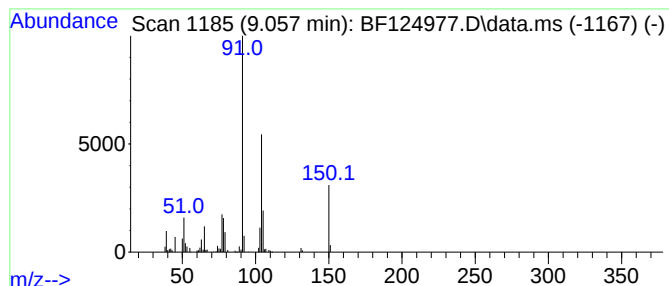
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hydrocinnamic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.057	111.48 ng	576436	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrocinnamic acid	150	C9H10O2	000501-52-0	96
2			4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	91
3			Benzenepropanoic acid, silver(1+...	256	C9H9AgO2	075112-79-7	59
4			2-Thiophenecarboxylic acid, 2-ph...	232	C13H12O2S	1000278-88-6	43
5			Propanoic acid, 2-methyl-, 2-phe...	192	C12H16O2	000103-48-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124977.D
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Instrument :
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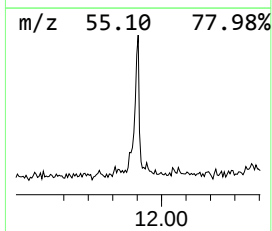
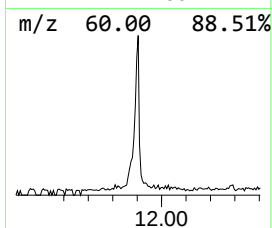
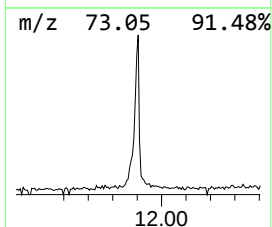
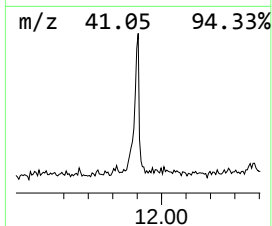
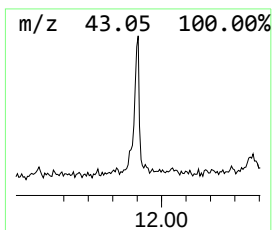
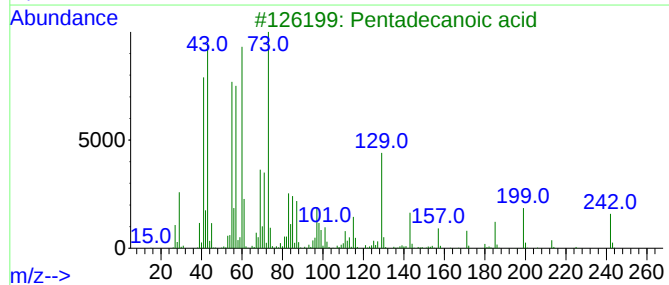
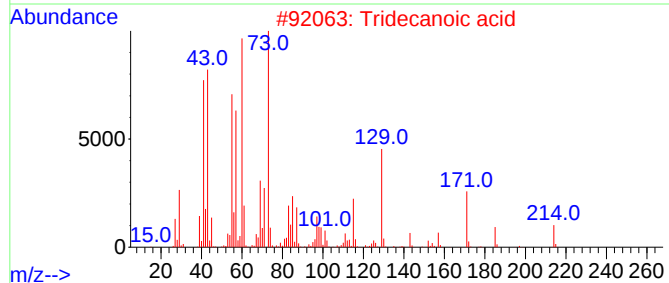
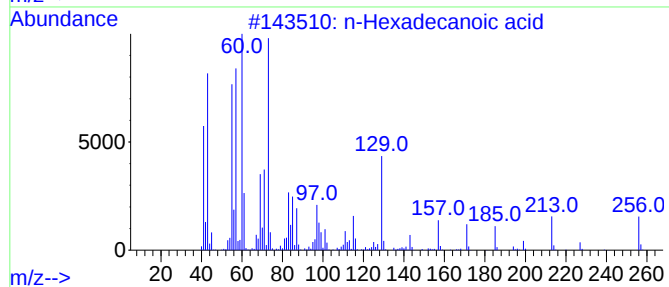
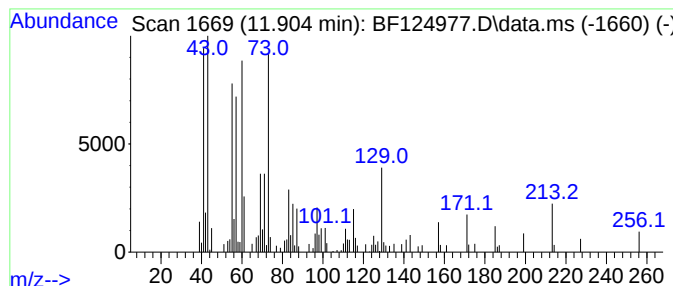
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	67.23 ng	193492	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	76
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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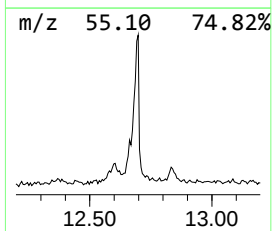
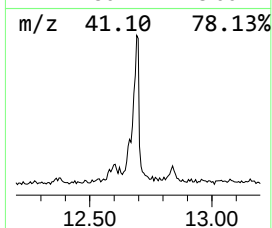
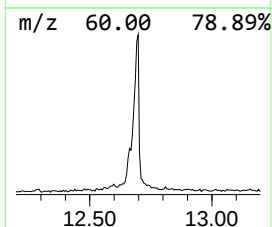
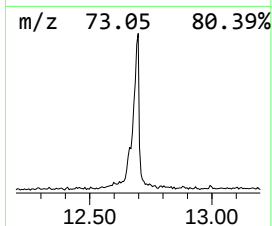
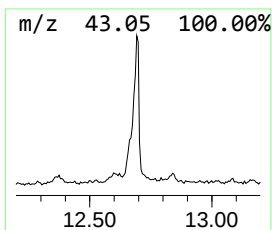
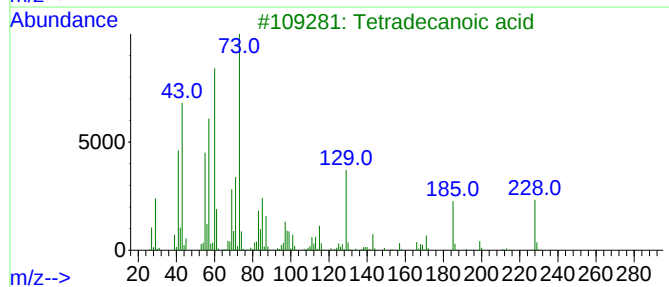
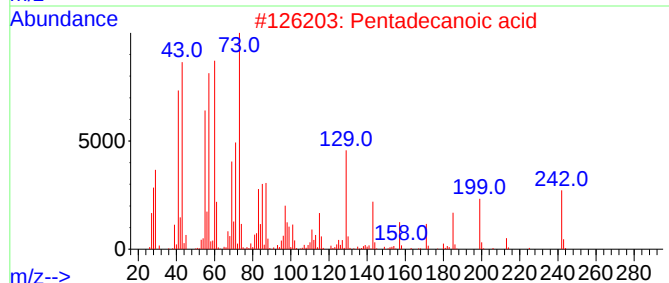
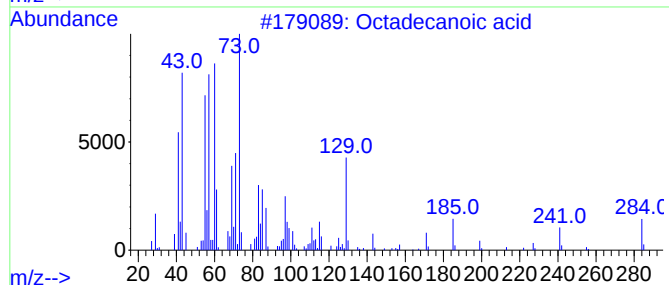
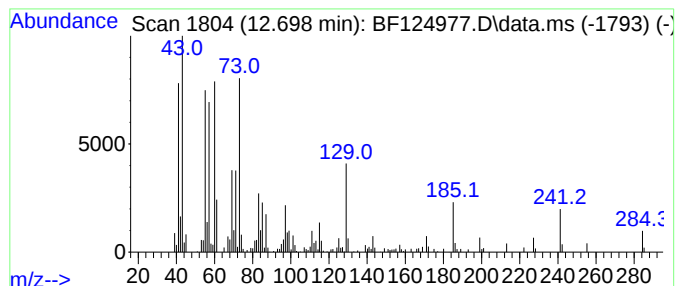
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	210.70 ng	462598	Chrysene-d12	13.992

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	53
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124977.D
Acq On : 7 Aug 2021 16:46
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Sample : M3297-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

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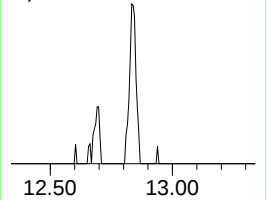
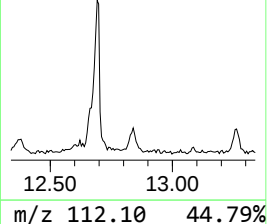
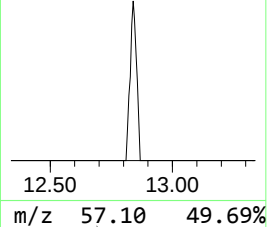
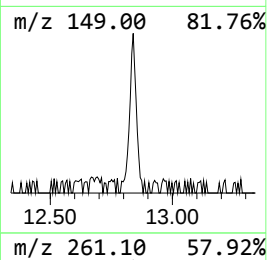
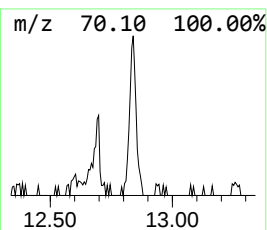
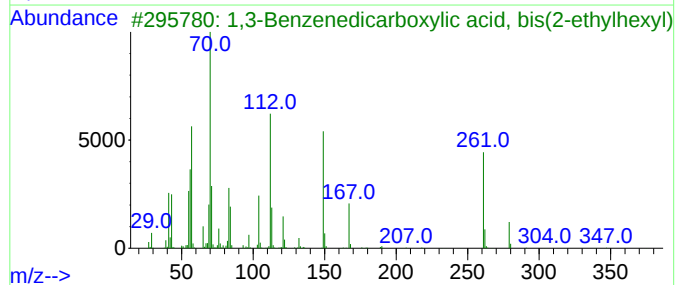
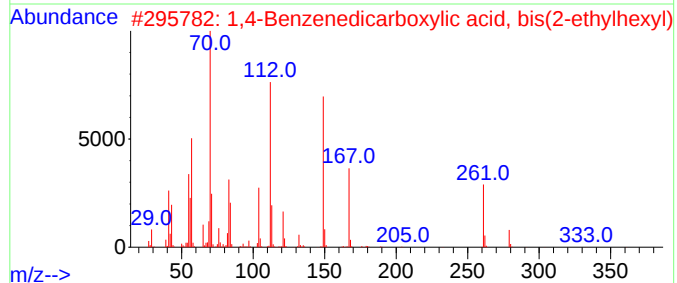
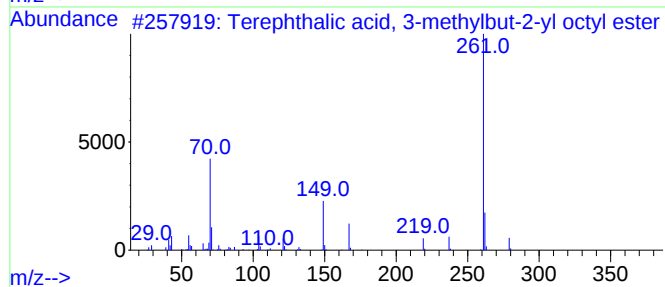
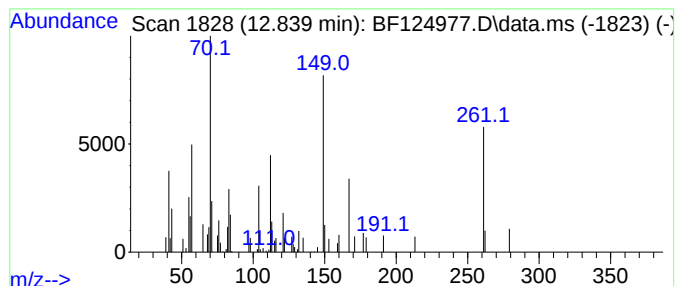
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Terephthalic acid, 3-methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.839	45.20 ng	99234	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	64
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	53
4			Terephthalic acid, dodec-2-enyl ...	444	C28H44O4	1000356-30-9	38
5			Terephthalic acid, 4-cyanophenyl...	379	C23H25NO4	1000323-66-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124977.D
Acq On : 7 Aug 2021 16:46
Operator : JU/CG
Sample : M3297-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
121

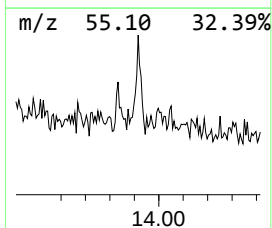
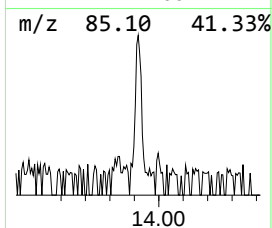
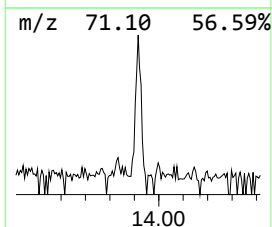
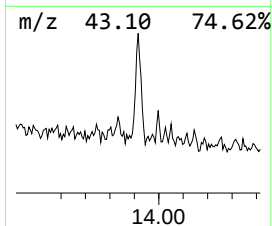
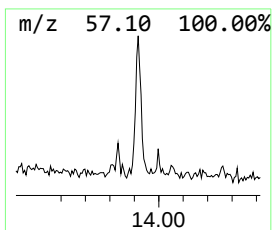
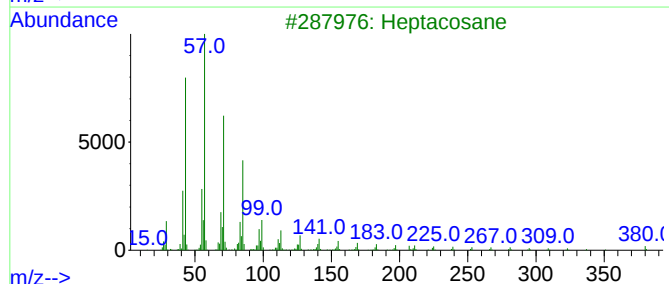
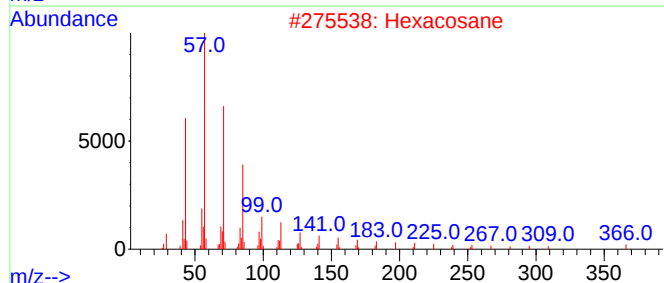
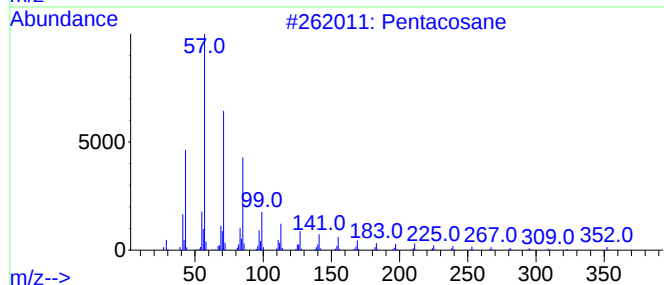
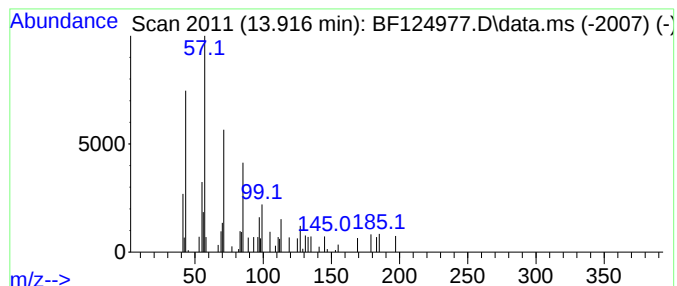
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Pentacosane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	23.51 ng	51620	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	90
2			Hexacosane	366	C26H54	000630-01-3	80
3			Heptacosane	380	C27H56	000593-49-7	80
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	64
5			Heptadecane	240	C17H36	000629-78-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124977.D
Acq On : 7 Aug 2021 16:46
Operator : JU/CG
Sample : M3297-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
121

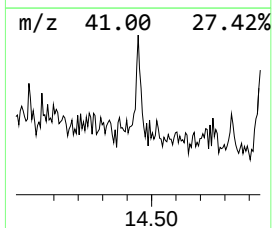
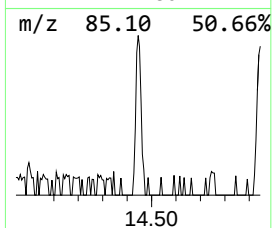
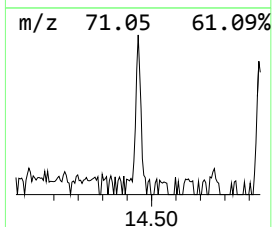
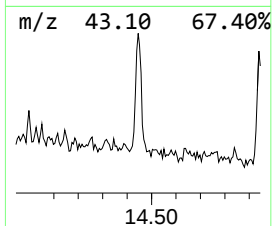
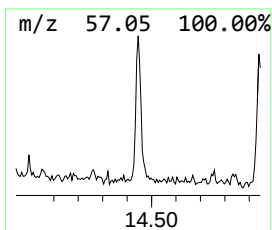
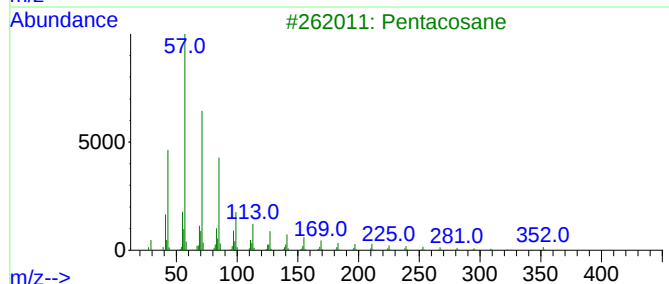
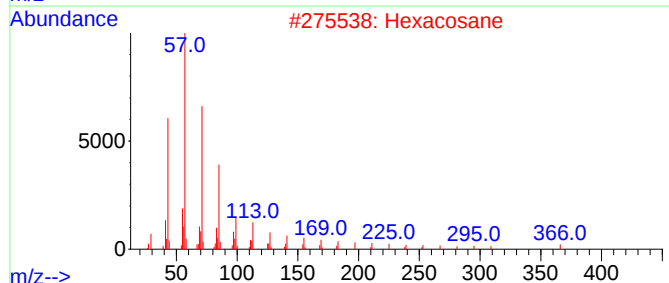
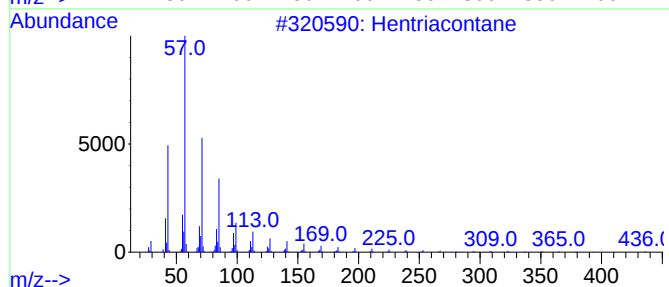
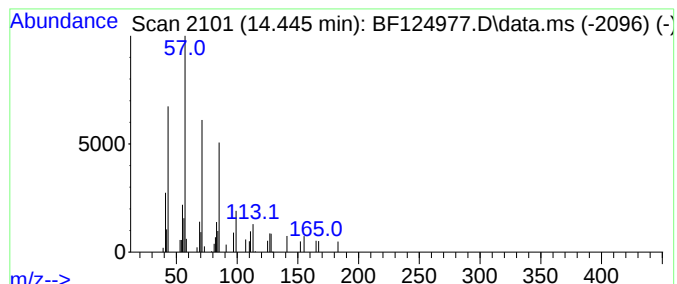
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Hentriacontane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	24.06 ng	52825	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Hexacosane	366	C26H54	000630-01-3	90
3			Pentacosane	352	C25H52	000629-99-2	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124977.D
Acq On : 7 Aug 2021 16:46
Operator : JU/CG
Sample : M3297-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
121

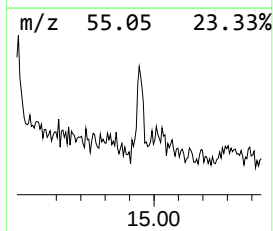
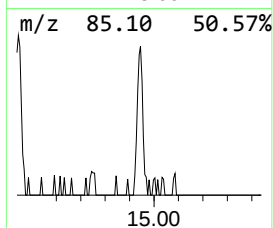
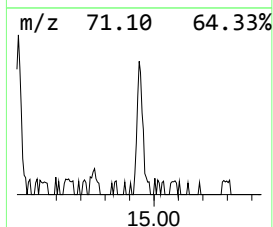
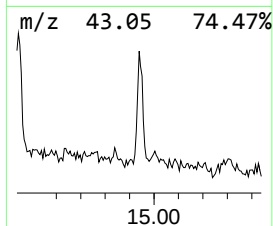
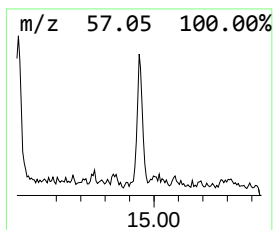
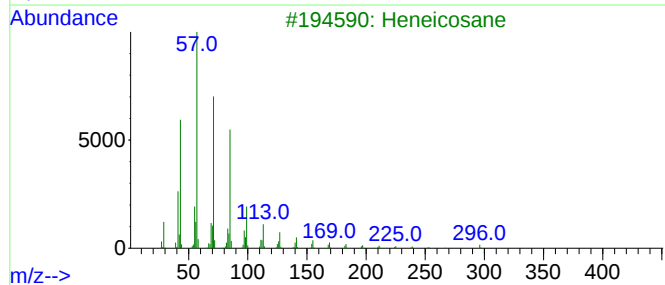
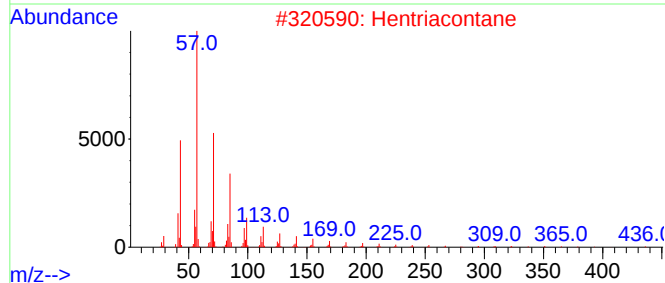
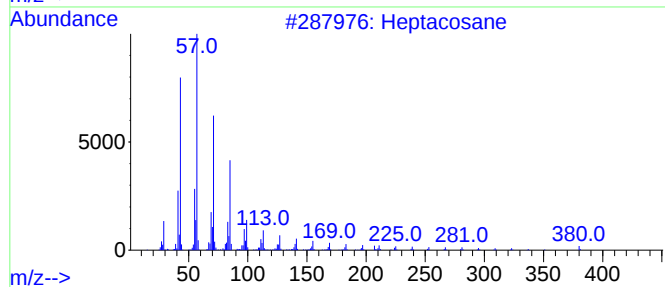
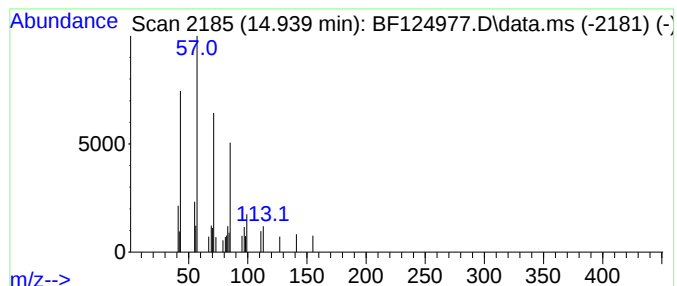
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Heptacosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	25.64 ng	44126	Perylene-d12	15.451

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5		Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
 Data File : BF124977.D
 Acq On : 7 Aug 2021 16:46
 Operator : JU/CG
 Sample : M3297-05
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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
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unknown5.934	5.934	22.0	ng	37824	1	6.828	34379	20.0
unknown6.381	6.381	27.1	ng	46559	1	6.828	34379	20.0
Hexanoic acid	6.592	24.0	ng	41193	1	6.828	34379	20.0
5-Methylhexanoi...	7.051	19.8	ng	34024	1	6.828	34379	20.0
Heptanoic acid	7.322	33.0	ng	56726	1	6.828	34379	20.0
unknown7.581	7.581	44.5	ng	94497	2	8.110	42487	20.0
Hexanoic acid, ...	7.775	471.2	ng	1000930	2	8.110	42487	20.0
Octanoic acid, ...	8.304	50.4	ng	107104	2	8.110	42487	20.0
Benzoic acid, 4...	8.469	67.9	ng	144167	2	8.110	42487	20.0
Benzeneacetic acid	8.569	290.2	ng	616497	2	8.110	42487	20.0
unknown8.816	8.816	29.8	ng	63346	2	8.110	42487	20.0
Nonanoic acid, ...	8.869	33.7	ng	71650	2	8.110	42487	20.0
Hydrocinnamic acid	9.057	111.5	ng	576436	3	9.869	103419	20.0
n-Hexadecanoic ...	11.904	67.2	ng	193492	4	11.351	57558	20.0
Octadecanoic acid	12.698	210.7	ng	462598	5	13.992	43911	20.0
Terephthalic ac...	12.839	45.2	ng	99234	5	13.992	43911	20.0
Pentacosane	13.916	23.5	ng	51620	5	13.992	43911	20.0
Hentriacontane	14.445	24.1	ng	52825	5	13.992	43911	20.0
Heptacosane	14.939	25.6	ng	44126	6	15.451	34420	20.0