

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
 Data File : BF134297.D
 Acq On : 14 Jul 2023 19:02
 Operator : CG\JU
 Sample : 03563-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HOUSE-BASEMENT

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-BF062623.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134297.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.916	308	311	320	rVB	30888	43693	2.49%	0.237%
2	5.063	503	506	516	rVB	45061	49052	2.80%	0.266%
3	5.469	571	575	590	rBV	520251	527462	30.10%	2.856%
4	6.146	688	690	701	rVB	27467	32325	1.84%	0.175%
5	6.475	742	746	756	rBV	370677	413414	23.59%	2.238%
6	6.551	756	759	764	rVB	69603	54804	3.13%	0.297%
7	6.616	767	770	778	rBV2	34283	37682	2.15%	0.204%
8	6.840	804	808	812	rBV	591773	474463	27.08%	2.569%
9	6.904	816	819	823	rBV2	20967	32263	1.84%	0.175%
10	7.034	838	841	844	rBV	121131	101307	5.78%	0.548%
11	7.245	873	877	888	rBV	144671	162233	9.26%	0.878%
12	7.404	900	904	907	rBV	1083559	890928	50.84%	4.823%
13	7.434	907	909	914	rVB3	32627	34283	1.96%	0.186%
14	7.545	925	928	932	rVB	72371	55851	3.19%	0.302%
15	7.640	942	944	949	rBV	52574	49205	2.81%	0.266%
16	7.804	967	972	975	rBV2	25842	27290	1.56%	0.148%
17	7.845	975	979	981	rVV	43025	43925	2.51%	0.238%
18	7.893	985	987	992	rVV2	21138	23797	1.36%	0.129%
19	8.028	1006	1010	1016	rBV	88302	119745	6.83%	0.648%
20	8.122	1022	1026	1033	rVB	735505	705367	40.25%	3.819%
21	8.240	1043	1046	1052	rVB	417407	338410	19.31%	1.832%
22	8.292	1052	1055	1060	rBV3	58966	101495	5.79%	0.549%
23	8.340	1060	1063	1065	rVV	74064	78279	4.47%	0.424%
24	8.369	1065	1068	1073	rVB2	66793	88575	5.05%	0.480%
25	8.716	1122	1127	1133	rBV	505149	647847	36.97%	3.507%
26	8.763	1133	1135	1143	rVB	89144	125480	7.16%	0.679%
27	8.992	1171	1174	1178	rBV	82023	71479	4.08%	0.387%
28	9.198	1205	1209	1212	rBV	2206146	1752398	100.00%	9.487%
29	9.310	1226	1228	1231	rVB	26992	22164	1.26%	0.120%
30	9.357	1231	1236	1241	rBV8	20179	40816	2.33%	0.221%
31	9.487	1253	1258	1261	rBV	59811	66358	3.79%	0.359%
32	9.751	1299	1303	1305	rBV	64760	58155	3.32%	0.315%
33	9.792	1308	1310	1315	rVV3	79533	84456	4.82%	0.457%
34	9.839	1315	1318	1321	rVV	211279	215940	12.32%	1.169%
35	9.881	1321	1325	1328	rVV	846860	843339	48.12%	4.566%
36	9.928	1331	1333	1335	rVV2	60483	61990	3.54%	0.336%

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Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	9.951	1335	1337	1342	rVB2	41414	53238	3.04%	0.288%
38	10.039	1350	1352	1357	rVB5	21277	24828	1.42%	0.134%
39	10.086	1357	1360	1364	rVB2	66218	69068	3.94%	0.374%
40	10.175	1373	1375	1378	rBV4	20116	25578	1.46%	0.138%
41	10.357	1403	1406	1410	rBV5	27145	46423	2.65%	0.251%
42	10.398	1410	1413	1417	rVV2	49204	65770	3.75%	0.356%
43	10.516	1430	1433	1437	rVB4	15045	22049	1.26%	0.119%
44	10.598	1443	1447	1451	rVB	431967	392737	22.41%	2.126%
45	10.675	1456	1460	1467	rBV	1026288	920479	52.53%	4.983%
46	10.739	1467	1471	1473	rBV	107845	102550	5.85%	0.555%
47	10.781	1475	1478	1480	rBV	44311	32661	1.86%	0.177%
48	10.810	1480	1483	1486	rBV	209503	168176	9.60%	0.911%
49	10.898	1496	1498	1502	rVB4	43173	48132	2.75%	0.261%
50	10.963	1507	1509	1515	rBV7	16735	28517	1.63%	0.154%
51	11.039	1519	1522	1527	rVB3	39164	31908	1.82%	0.173%
52	11.175	1541	1545	1548	rBV5	22435	42574	2.43%	0.230%
53	11.204	1548	1550	1553	rVV2	70478	74171	4.23%	0.402%
54	11.239	1553	1556	1559	rVV4	39562	59446	3.39%	0.322%
55	11.298	1562	1566	1569	rVV2	46855	73729	4.21%	0.399%
56	11.328	1569	1571	1573	rVB2	38219	30546	1.74%	0.165%
57	11.375	1575	1579	1586	rVB	868675	721528	41.17%	3.906%
58	11.428	1586	1588	1590	rBV2	31506	27289	1.56%	0.148%
59	11.504	1598	1601	1603	rVB	25679	22438	1.28%	0.121%
60	11.545	1604	1608	1613	rBV2	125092	165686	9.45%	0.897%
61	11.628	1616	1622	1625	rVV4	51304	91982	5.25%	0.498%
62	11.698	1631	1634	1636	rVB	61315	55393	3.16%	0.300%
63	11.792	1646	1650	1651	rBV3	27169	27829	1.59%	0.151%
64	11.839	1654	1658	1666	rVV2	173378	212280	12.11%	1.149%
65	11.916	1666	1671	1680	rVV	1020184	1146706	65.44%	6.208%
66	12.316	1736	1739	1740	rBV3	39741	40245	2.30%	0.218%
67	12.469	1761	1765	1769	rVB2	71690	77786	4.44%	0.421%
68	12.622	1788	1791	1792	rBV2	57171	57123	3.26%	0.309%
69	12.698	1801	1804	1817	rVB2	243196	321848	18.37%	1.742%
70	12.892	1834	1837	1841	rVB	77240	70022	4.00%	0.379%
71	12.975	1846	1851	1854	rBV	1859297	1750669	99.90%	9.478%
72	13.198	1887	1889	1894	rBV2	45730	57534	3.28%	0.311%
73	13.533	1943	1946	1951	rBV2	91486	93747	5.35%	0.508%
74	13.886	2001	2006	2024	rBV5	261904	659261	37.62%	3.569%
75	14.010	2024	2027	2029	rVV	75990	74700	4.26%	0.404%
76	14.033	2029	2031	2038	rVB	579774	573779	32.74%	3.106%

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77	14.192	2056	2058	2061	rVB	55109	45816	2.61%	0.248%
78	14.421	2094	2097	2100	rBV2	36580	43891	2.50%	0.238%
79	14.504	2107	2111	2114	rBV	66815	71671	4.09%	0.388%
80	14.710	2143	2146	2151	rVB	80897	83784	4.78%	0.454%
81	14.816	2161	2164	2169	rVB	68194	79443	4.53%	0.430%
82	14.892	2174	2177	2182	rVB2	62874	71702	4.09%	0.388%
83	15.169	2220	2224	2227	rVB	47494	51918	2.96%	0.281%
84	15.539	2282	2287	2300	rVB	373714	536706	30.63%	2.906%
85	16.021	2366	2369	2374	rVB2	22236	29816	1.70%	0.161%
86	16.486	2442	2448	2455	rBV2	42587	135031	7.71%	0.731%
87	16.586	2458	2465	2480	rVB9	52875	222231	12.68%	1.203%
88	16.751	2488	2493	2498	rVB8	31222	61943	3.53%	0.335%

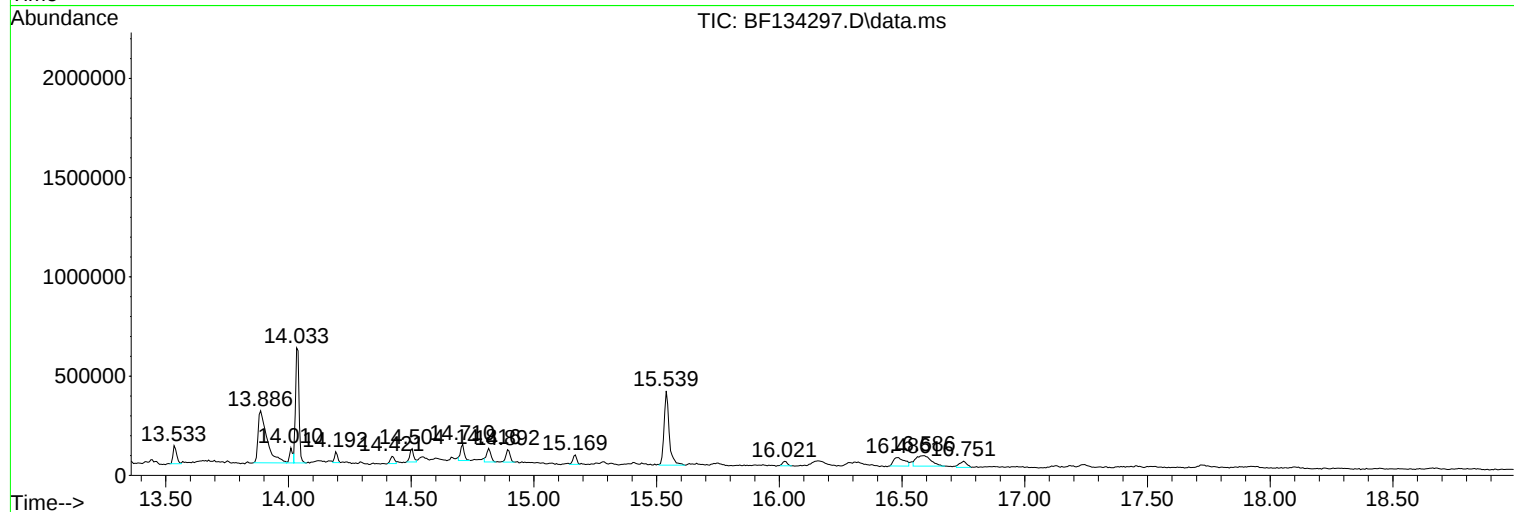
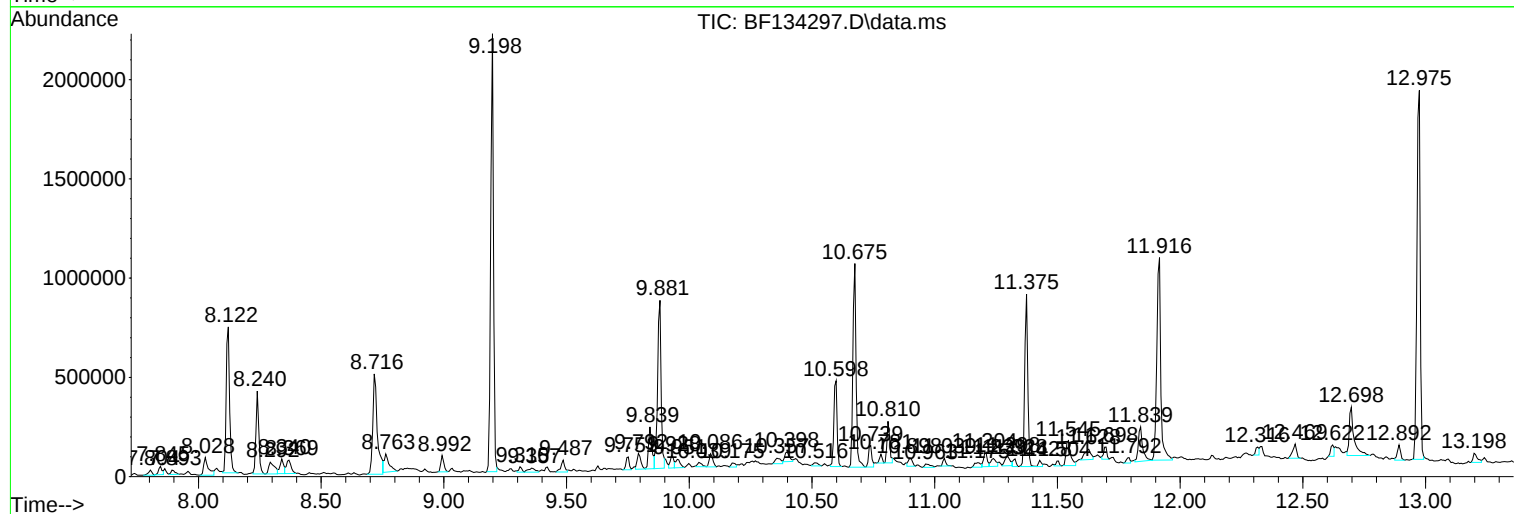
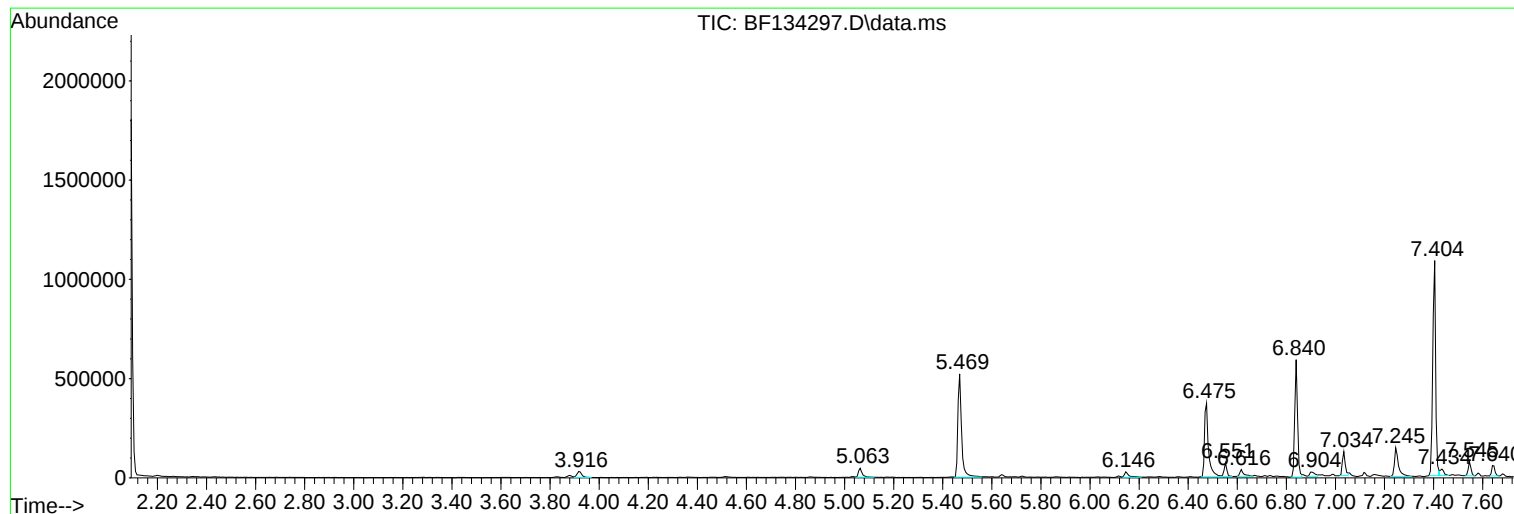
Sum of corrected areas: 18470647

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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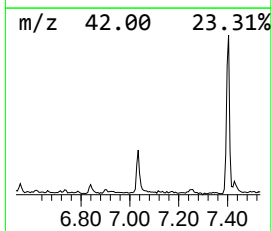
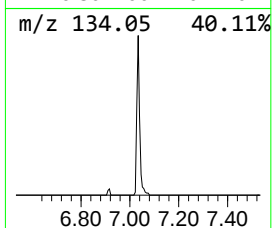
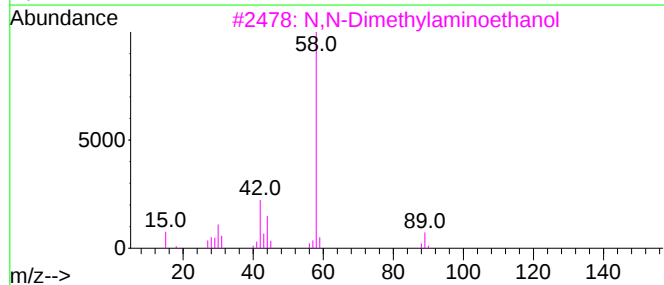
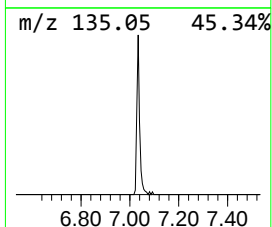
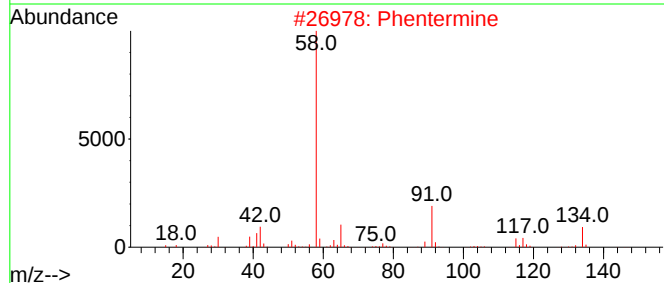
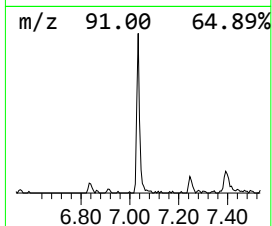
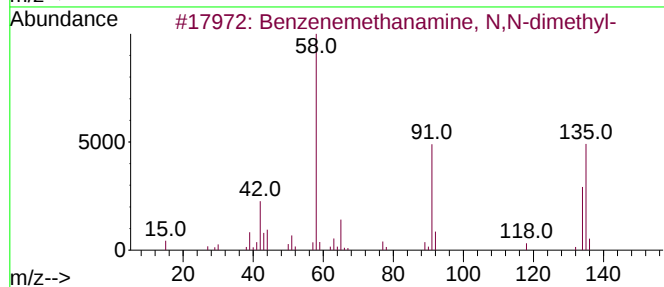
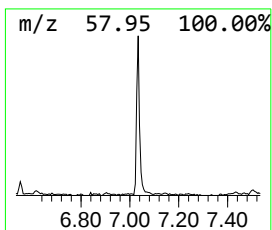
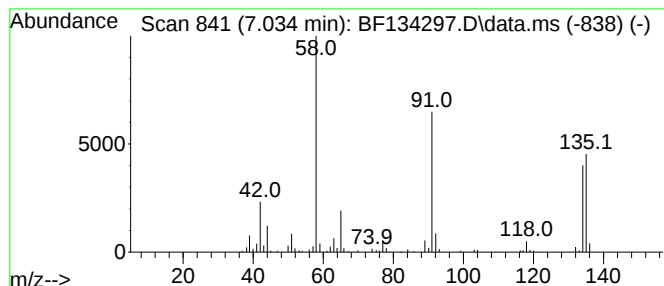
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzenemethanamine, N,N-dim... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.034	4.27 ng	101307	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenemethanamine, N,N-dimethyl-	135	C9H13N	000103-83-3	94
2			Phentermine	149	C10H15N	000122-09-8	53
3			N,N-Dimethylaminoethanol	89	C4H11NO	000108-01-0	35
4			2-(benzo[d][1,3]dioxol-5-yl)-N,N...	193	C11H15NO2	1000455-58-7	35
5			Benzene, (2-methoxyethenyl)-	134	C9H10O	004747-15-3	30



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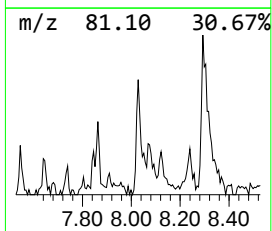
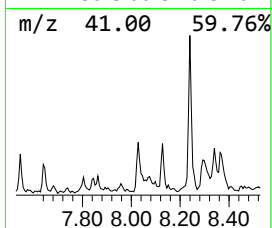
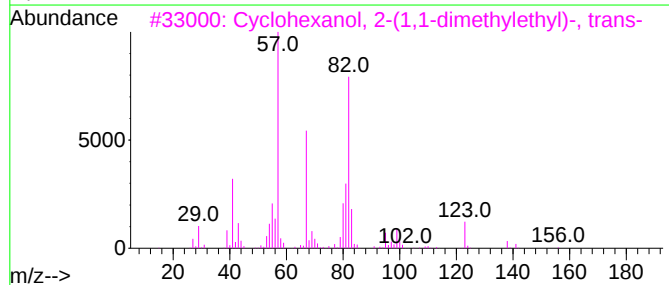
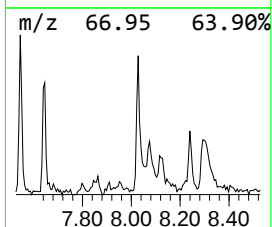
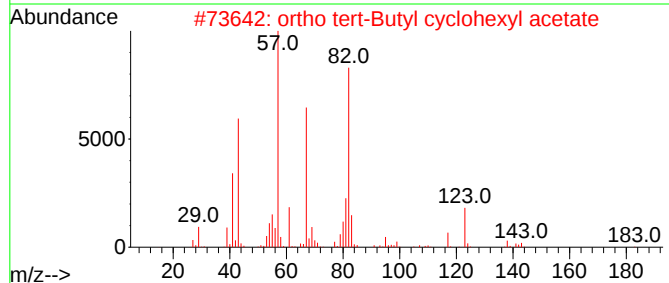
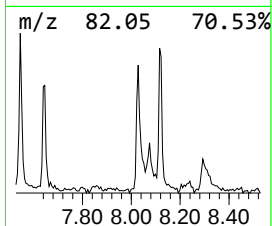
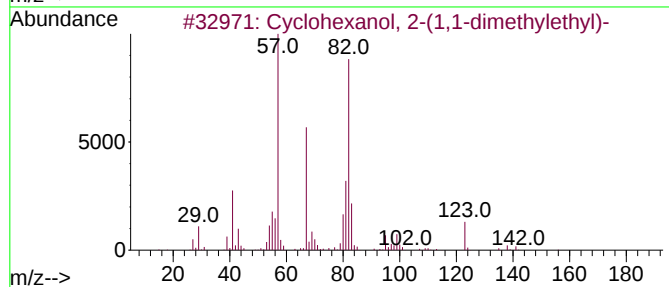
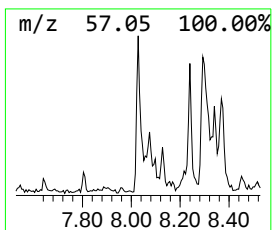
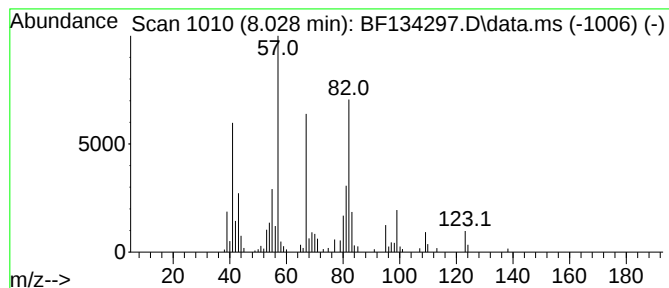
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexanol, 2-(1,1-dimeth... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.028	3.40 ng	119745	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanol, 2-(1,1-dimethyleth...	156	C10H20O	013491-79-7	59
2			ortho tert-Butyl cyclohexyl acetate	198	C12H22O2	000088-41-5	59
3			Cyclohexanol, 2-(1,1-dimethyleth...	156	C10H20O	005448-22-6	50
4			3-Octyne, 2-methyl-	124	C9H16	055402-15-8	43
5			Cyclohexanol, 2-(1,1-dimethyleth...	156	C10H20O	007214-18-8	43



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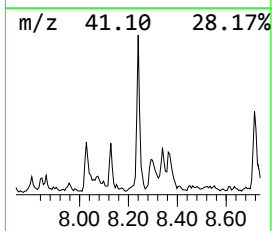
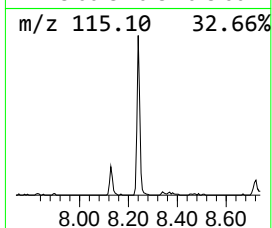
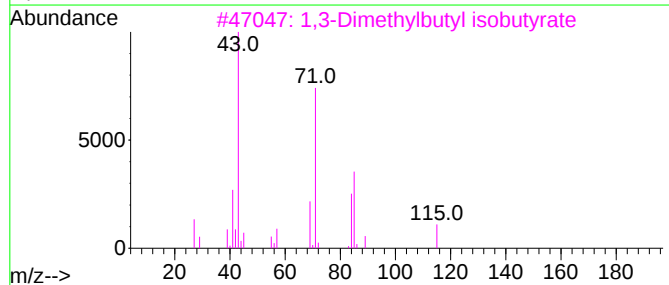
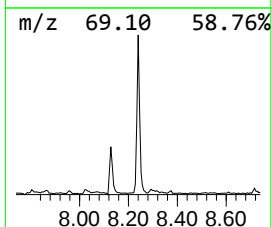
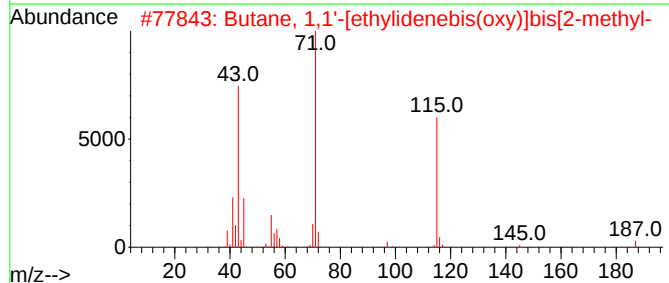
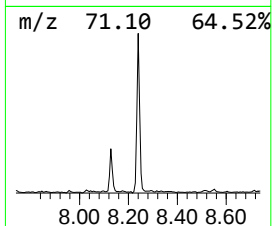
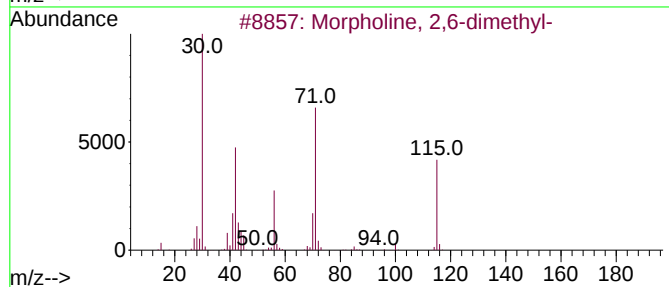
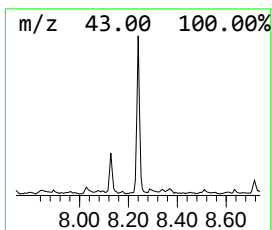
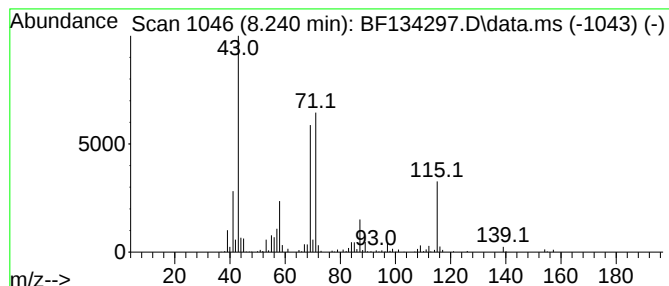
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.240 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.240	9.60 ng	338410	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	38
2			Butane, 1,1'-[ethylidenebis(oxy)...	202	C12H26O2	013535-43-8	37
3			1,3-Dimethylbutyl isobutyrate	172	C10H20O2	1000429-31-6	35
4			2,3'-Bifuran, octahydro-	142	C8H14O2	073373-15-6	35
5			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	27



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HOUSE-BASEMENT

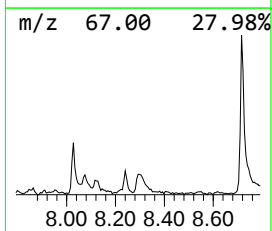
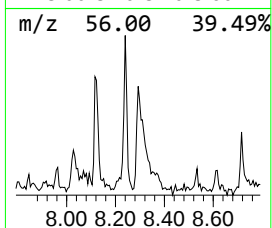
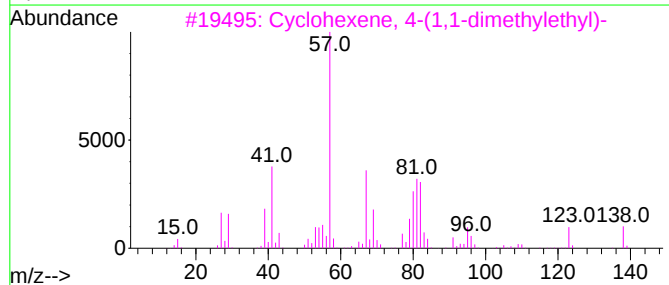
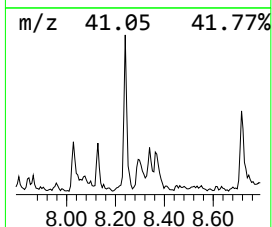
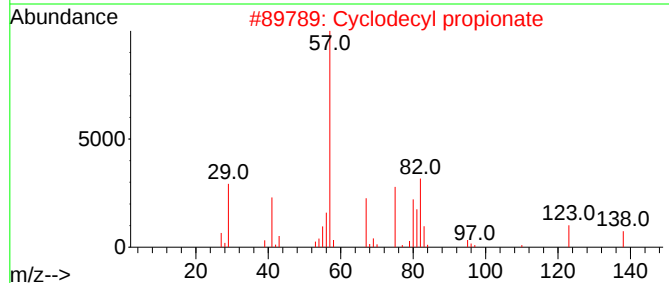
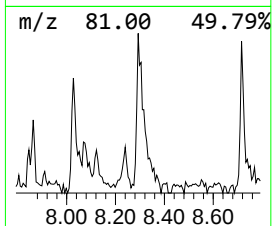
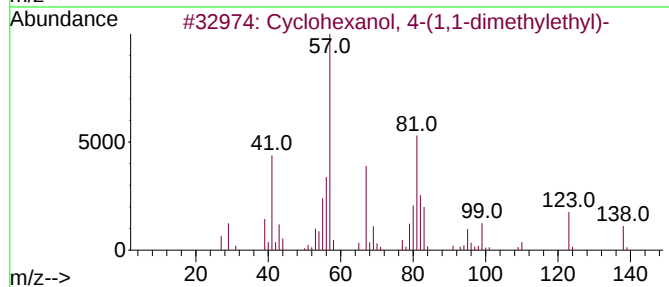
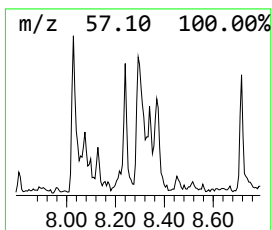
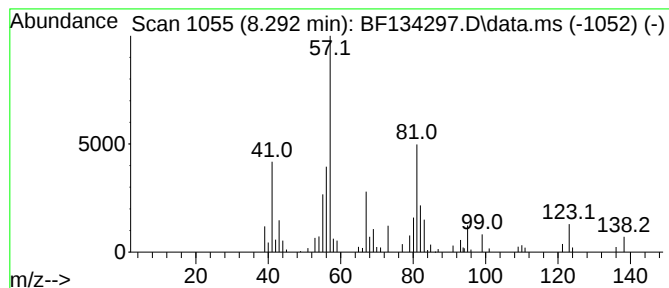
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclohexanol, 4-(1,1-dimeth... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.292	2.88 ng	101495	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanol, 4-(1,1-dimethyleth...	156	C10H20O	000098-52-2	58
2			Cyclodecyl propionate	212	C13H24O2	1000429-26-1	43
3			Cyclohexene, 4-(1,1-dimethylethyl)-	138	C10H18	002228-98-0	43
4			Cyclohexanol, 4-(1,1-dimethyleth...	156	C10H20O	021862-63-5	42
5			Cyclohexanol, 4-(1,1-dimethyleth...	198	C12H22O2	010411-92-4	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134297.D
Acq On : 14 Jul 2023 19:02
Operator : CG\JU
Sample : 03563-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HOUSE-BASEMENT

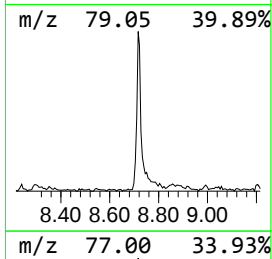
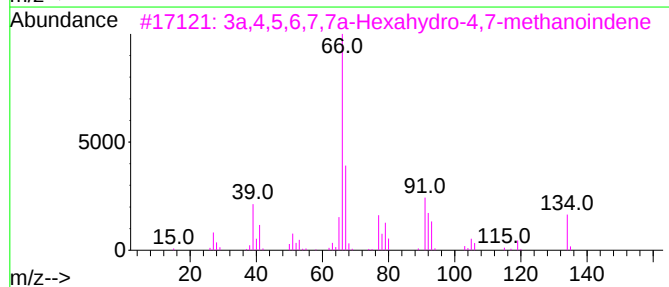
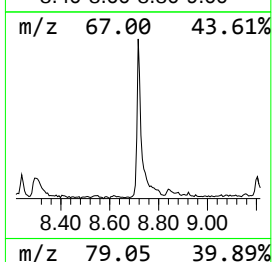
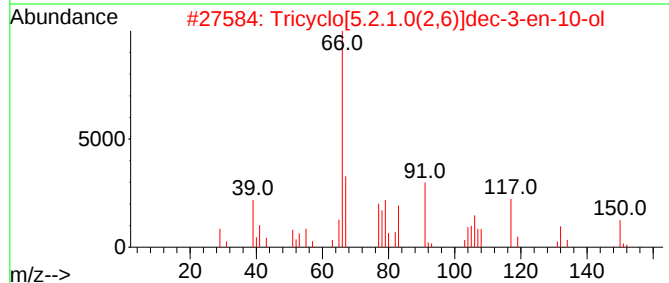
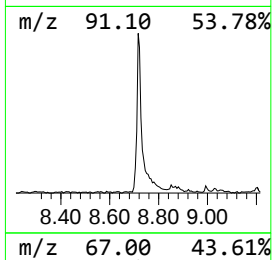
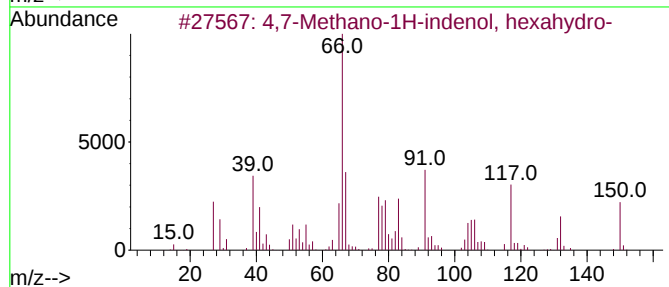
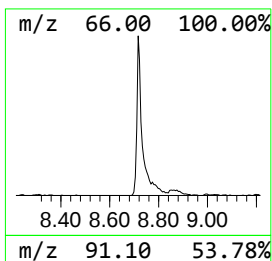
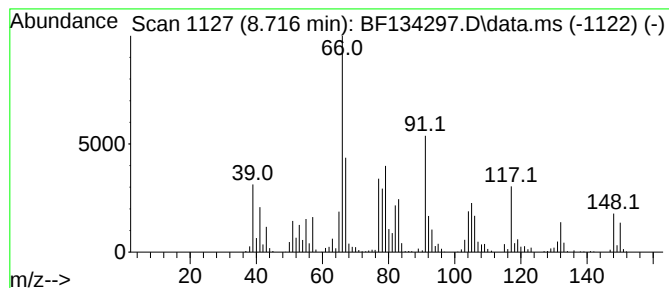
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4,7-Methano-1H-indenol, hex... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.716	18.37 ng	647847	Naphthalene-d8	8.122

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4,7-Methano-1H-indenol, hexahydro-	150	C10H14O	037275-49-3	95
2		Tricyclo[5.2.1.0(2,6)]dec-3-en-1...	150	C10H14O	039852-87-4	90
3		3a,4,5,6,7,7a-Hexahydro-4,7-meth...	134	C10H14	004488-57-7	72
4		Bicyclo[3.2.0]hept-2-ene, 6-meth...	106	C8H10	038695-51-1	59
5		Bicyclo[2.2.1]hept-2-ene, 5-meth...	106	C8H10	000694-91-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134297.D
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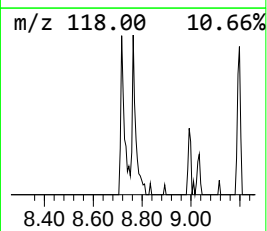
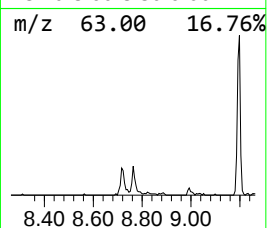
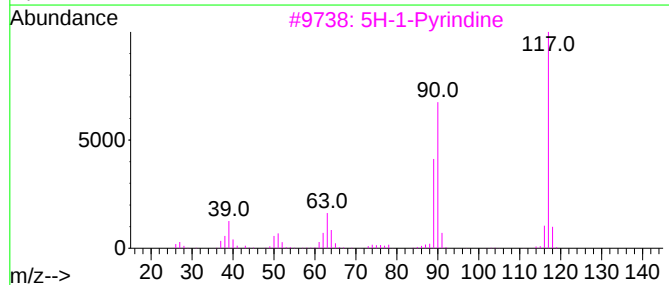
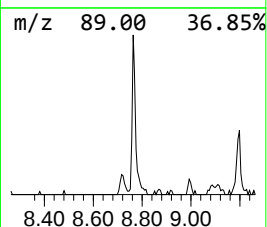
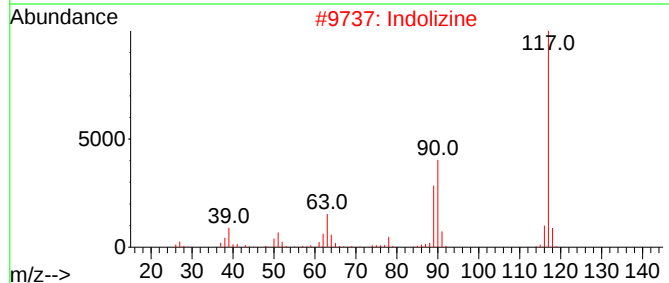
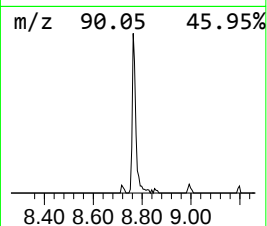
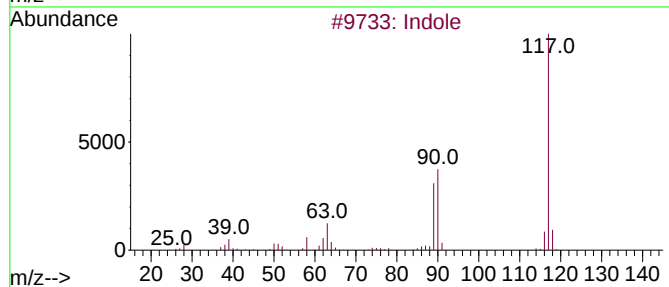
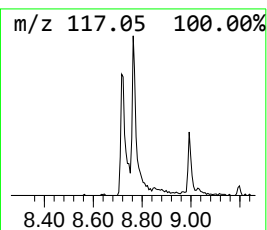
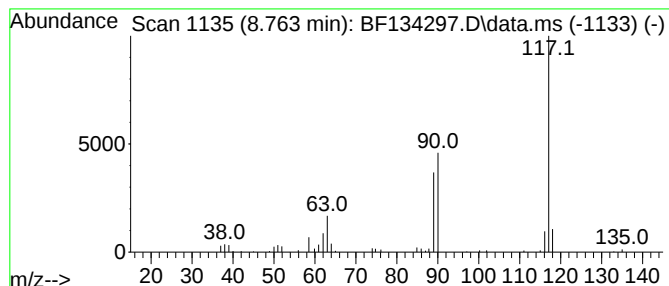
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Indole Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.763	3.56 ng	125480	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	94
2			Indolizine	117	C8H7N	000274-40-8	91
3			5H-1-Pyridine	117	C8H7N	000270-91-7	91
4			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	87
5			Benzyl nitrile	117	C8H7N	000140-29-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134297.D
Acq On : 14 Jul 2023 19:02
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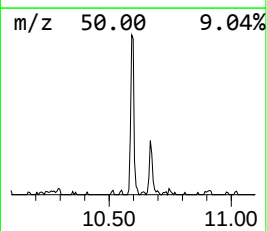
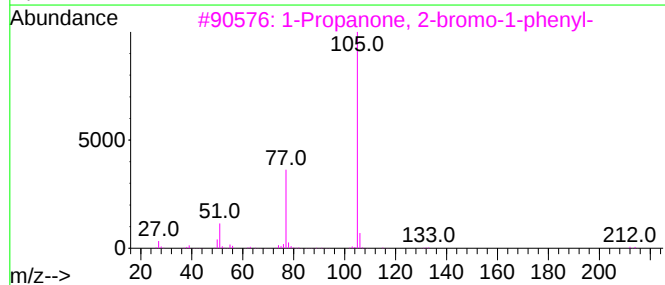
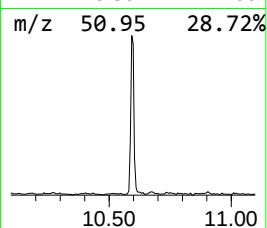
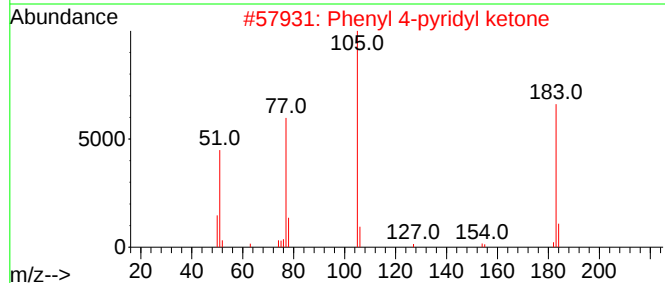
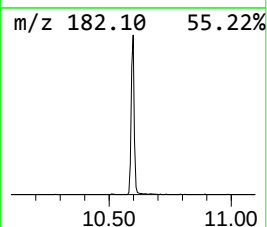
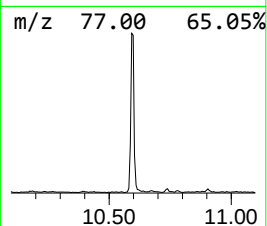
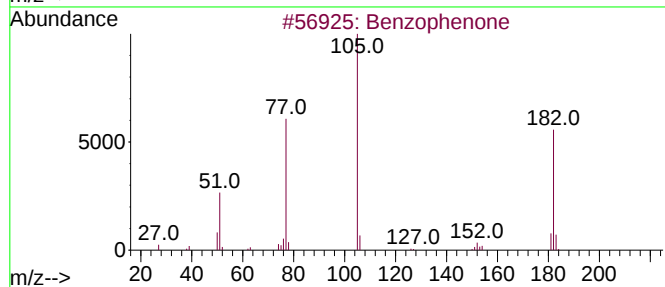
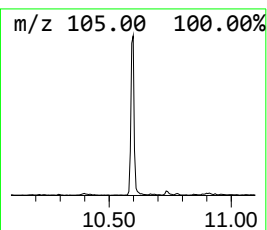
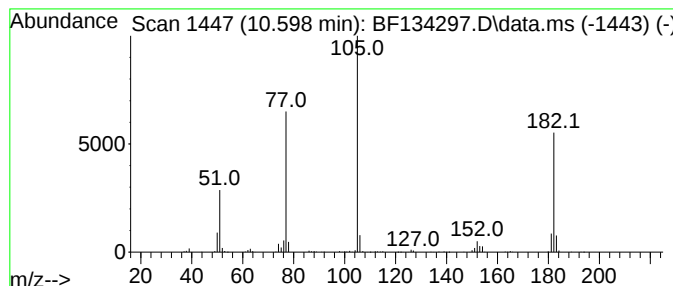
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	9.31 ng	392737	Acenaphthene-d10	9.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	50
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
5			N-cyanobenzamide	146	C8H6N2O	015150-25-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
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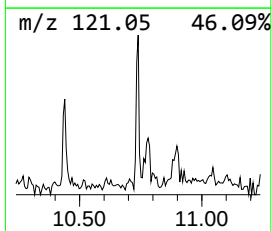
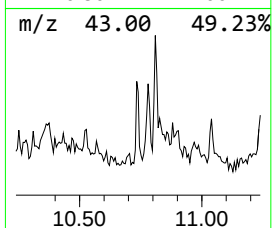
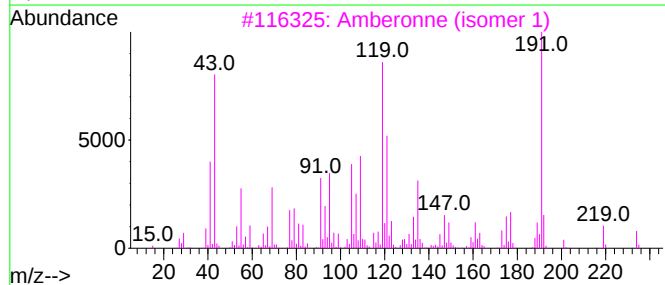
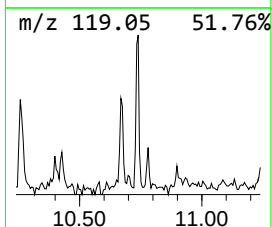
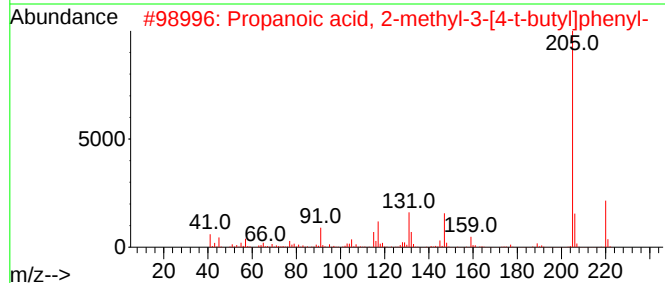
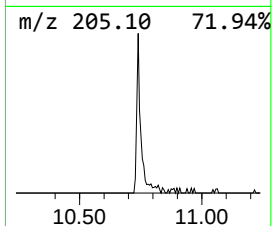
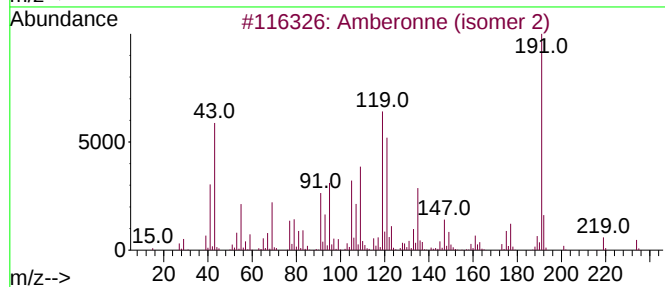
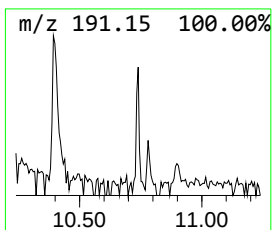
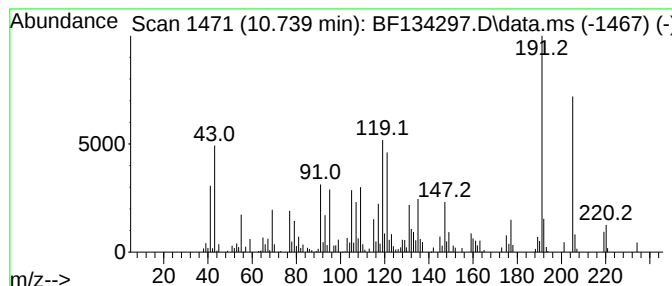
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Amberonne (isomer 2) Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	2.84 ng	102550	Phenanthrene-d10	11.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amberonne (isomer 2)	234	C16H26O	1010470-69-8	99
2			Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	83
3			Amberonne (isomer 1)	234	C16H26O	1000470-69-7	66
4			Propanoic acid, 2-[4-(1-formylet...	220	C13H16O3	1000161-46-8	53
5			2-(4-Methyl-1-piperazinyl)aniline	191	C11H17N3	180605-36-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
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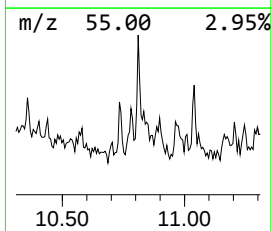
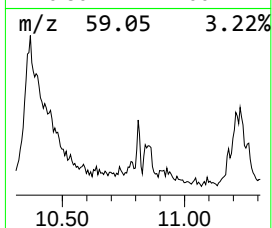
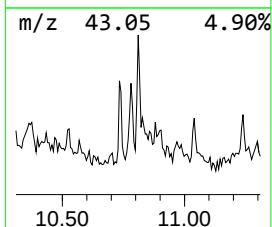
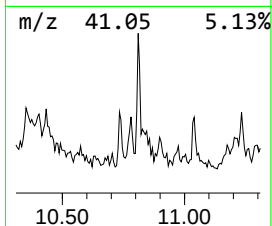
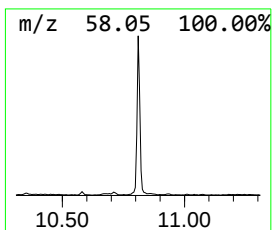
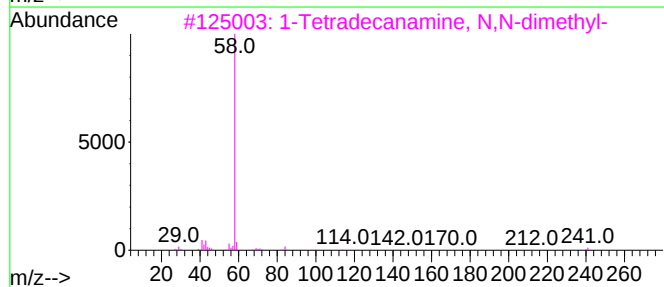
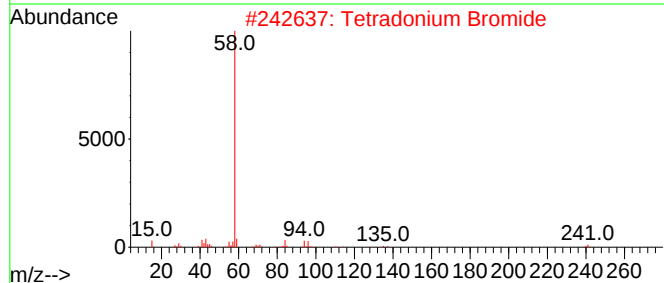
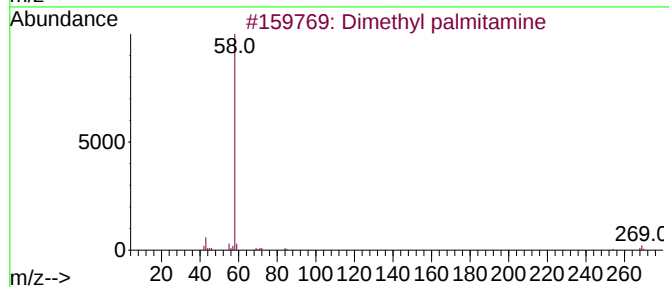
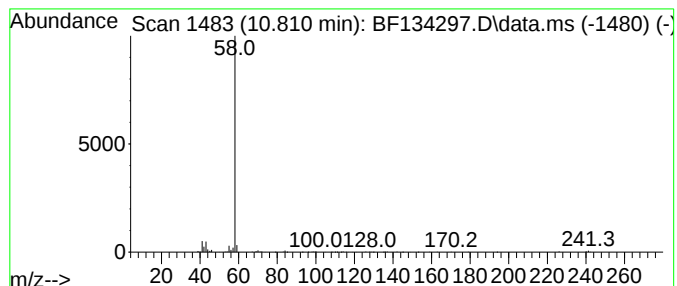
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dimethyl palmitamine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.810	4.66 ng	168176	Phenanthrene-d10	11.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl palmitamine	269	C18H39N	000112-69-6	72
2			Tetradonium Bromide	335	C17H38BrN	001119-97-7	72
3			1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	72
4			Cetrimonium Bromide	363	C19H42BrN	000057-09-0	56
5			Dimantine	297	C20H43N	000124-28-7	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
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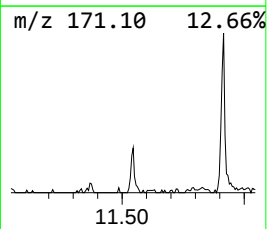
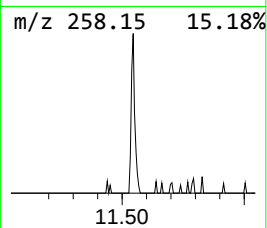
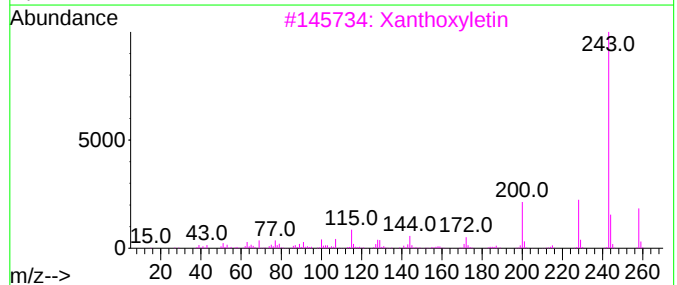
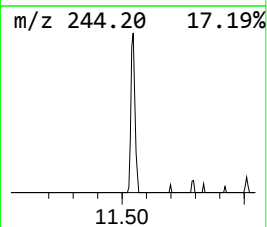
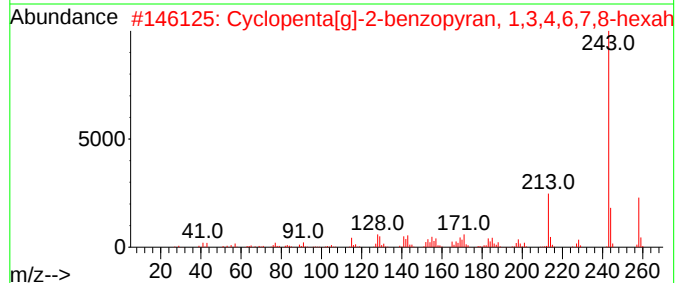
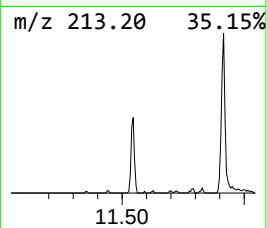
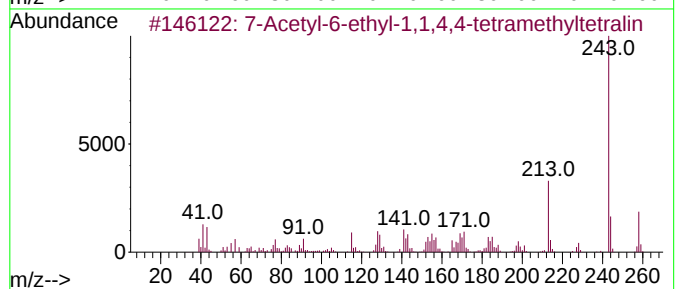
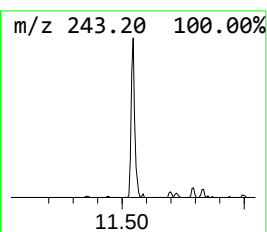
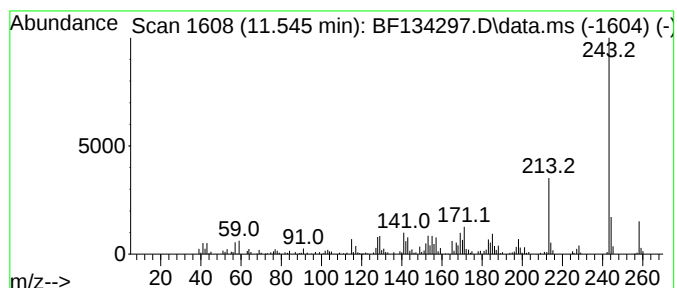
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HOUSE-BASEMENT

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 7-Acetyl-6-ethyl-1,1,4,4-te... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.545	4.59 ng	165686	Phenanthrene-d10		11.375	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7-Acetyl-6-ethyl-1,1,4,4-tetrame...		258	C18H26O	000088-29-9	99
2	Cyclopenta[g]-2-benzopyran, 1,3,...		258	C18H26O	001222-05-5	98
3	Xanthoxyletin		258	C15H14O4	000084-99-1	52
4	8-Methoxy-1,3,4,4a,5,6-hexahydro...		243	C15H17NO2	197661-85-1	50
5	6-Chrysenamine		243	C18H13N	002642-98-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134297.D
Acq On : 14 Jul 2023 19:02
Operator : CG\JU
Sample : 03563-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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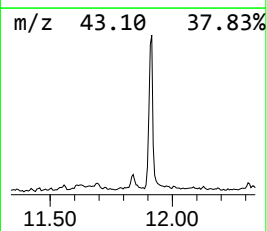
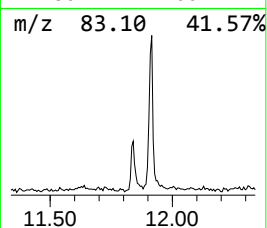
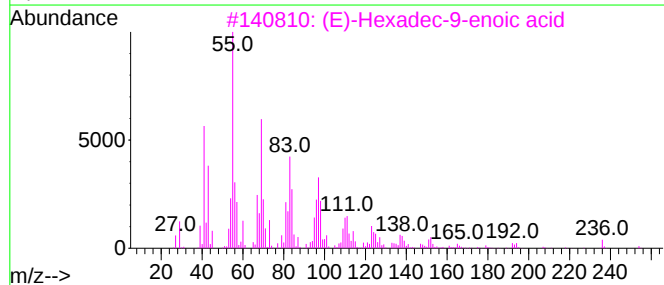
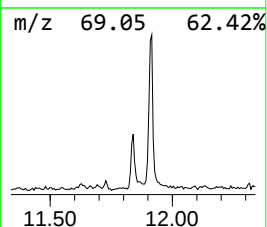
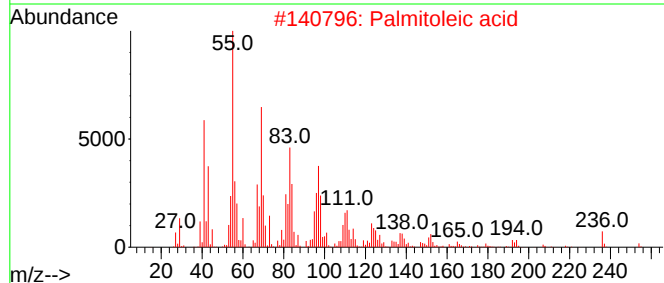
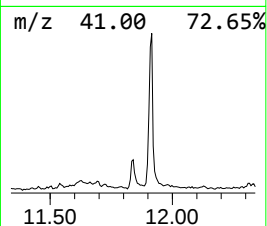
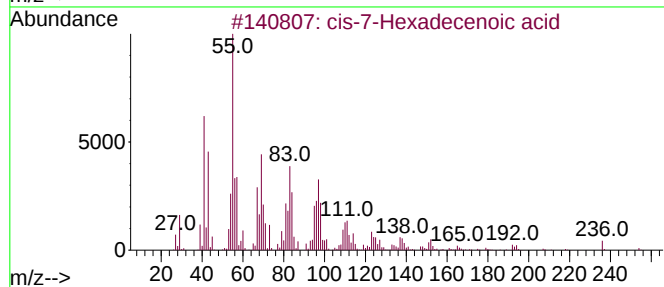
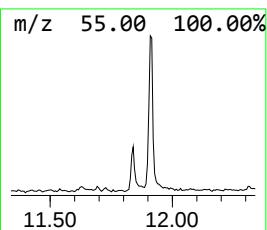
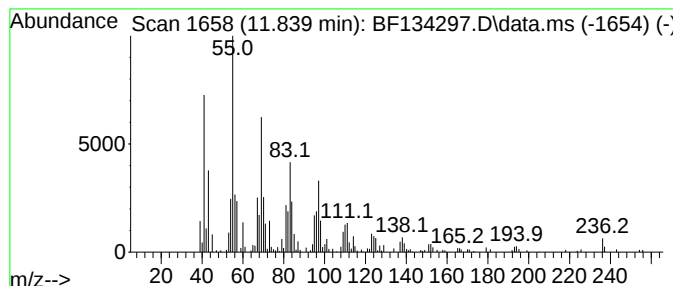
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 cis-7-Hexadecenoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	5.88 ng	212280	Phenanthrene-d10	11.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	97
2			Palmitoleic acid	254	C16H30O2	000373-49-9	97
3			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	96
4			6-Pentadecenoic acid, 13-methyl-...	254	C16H30O2	682751-34-4	95
5			Z-8-Hexadecene	224	C16H32	1000130-87-5	92



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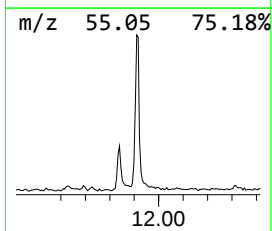
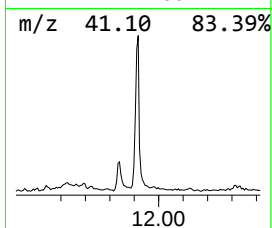
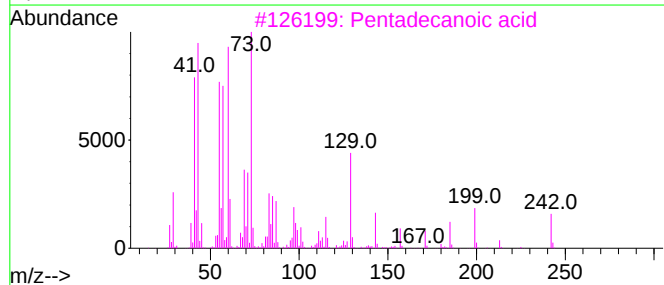
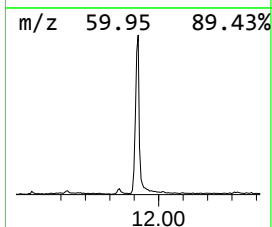
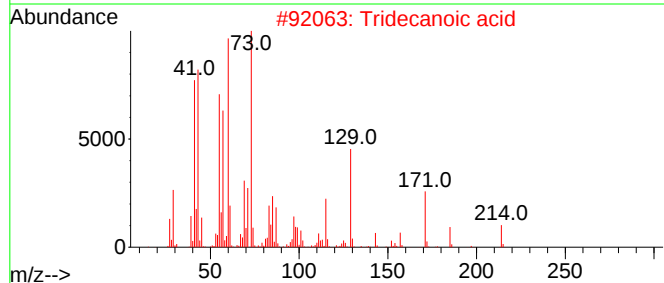
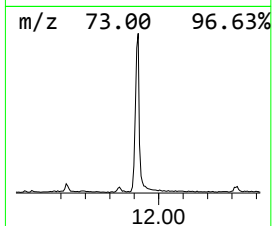
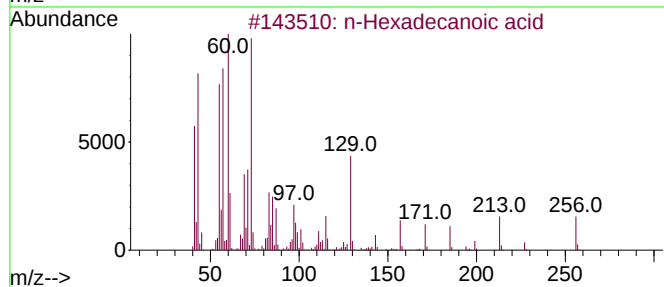
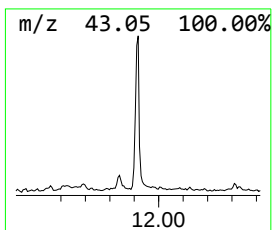
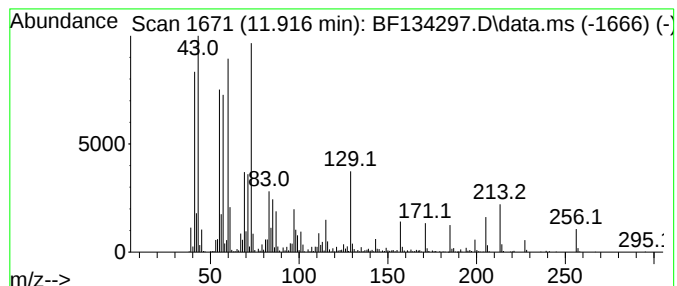
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	31.79 ng	1146710	Phenanthrene-d10	11.375

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Undecanoic acid	186	C11H22O2	000112-37-8	70
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
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Acq On : 14 Jul 2023 19:02
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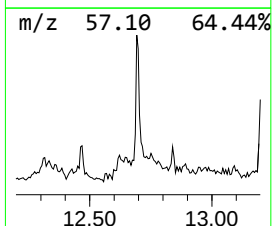
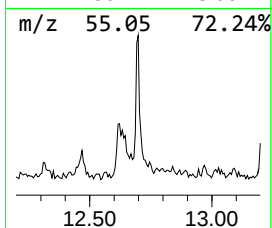
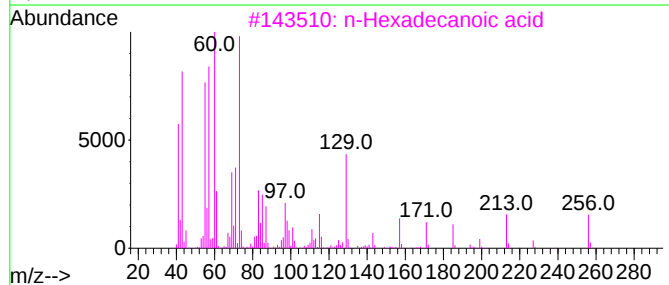
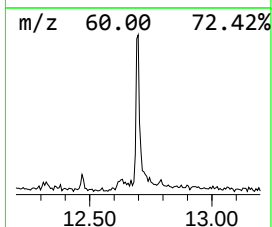
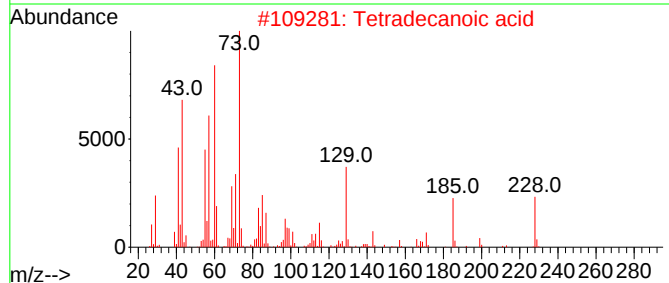
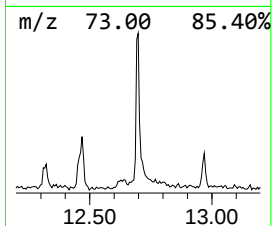
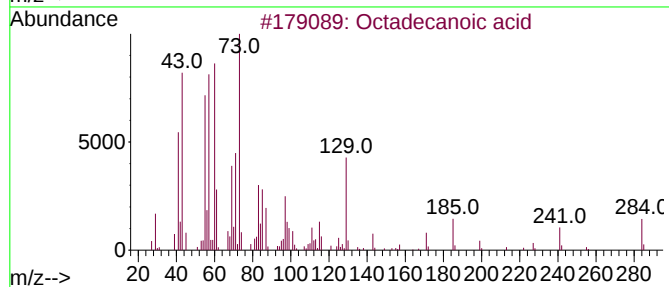
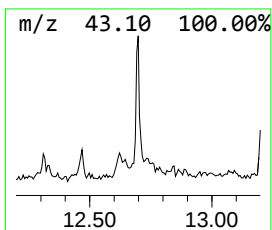
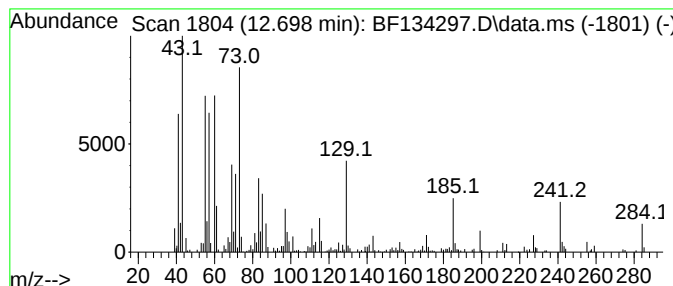
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.698	8.92 ng	321848	Phenanthrene-d10		11.375	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	91
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	74
3	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	62
4	n-Decanoic acid		172	C10H20O2	000334-48-5	45
5	Pentadecanoic acid		242	C15H30O2	001002-84-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134297.D
Acq On : 14 Jul 2023 19:02
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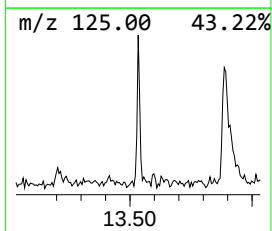
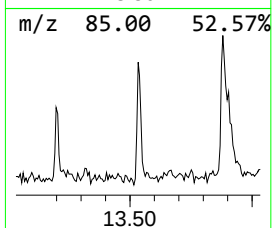
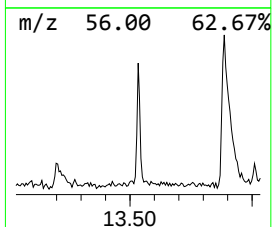
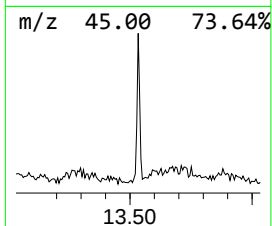
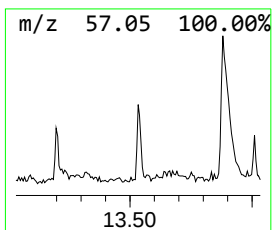
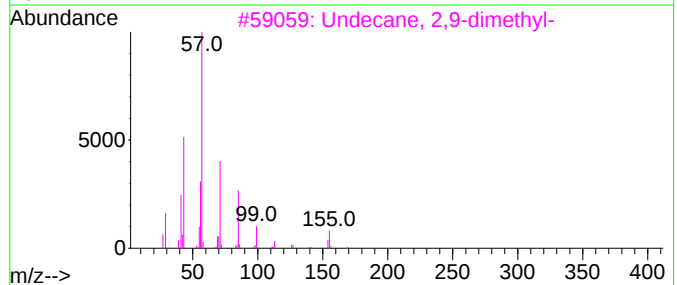
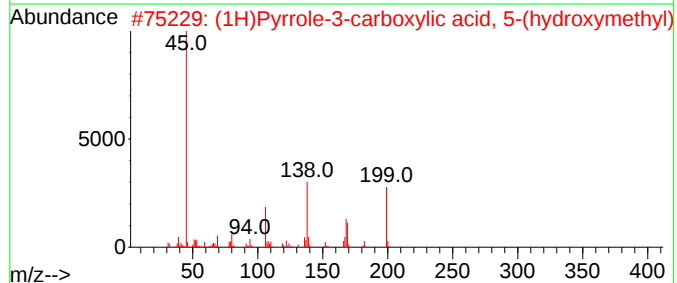
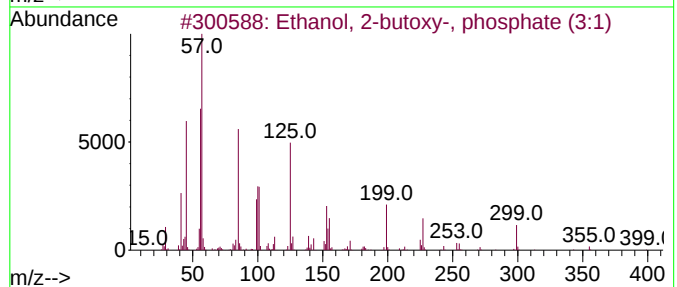
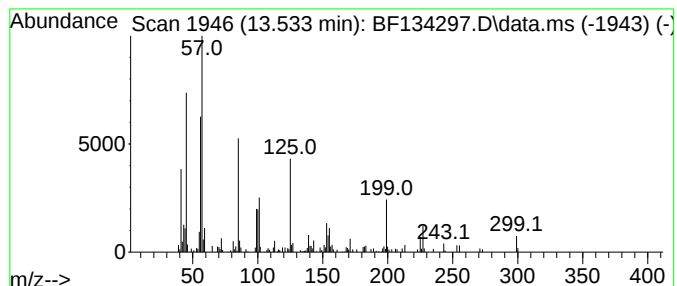
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Ethanol, 2-butoxy-, phospho... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.533	3.27 ng	93747	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	81
2			(1H)Pyrrole-3-carboxylic acid, 5...	199	C9H13NO4	155345-20-3	18
3			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	12
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	12
5			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	12



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Acq On : 14 Jul 2023 19:02
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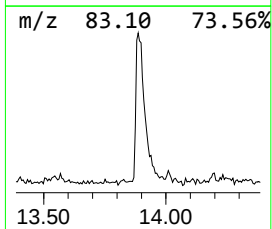
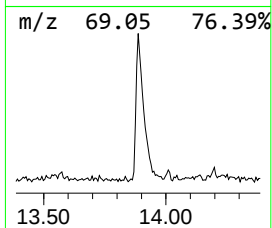
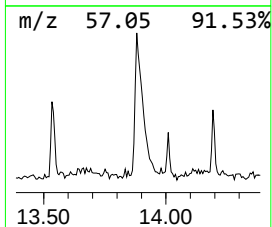
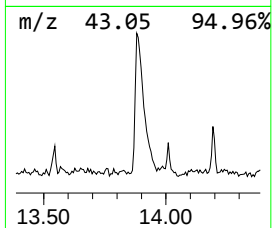
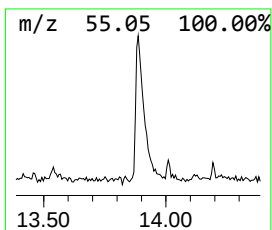
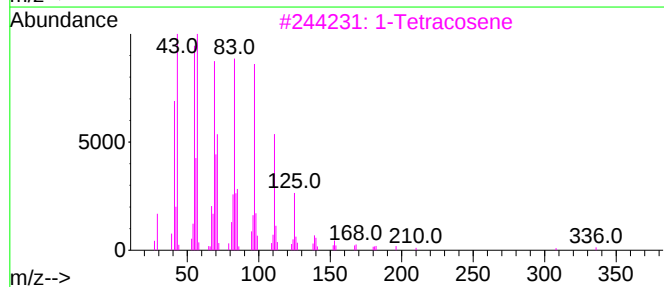
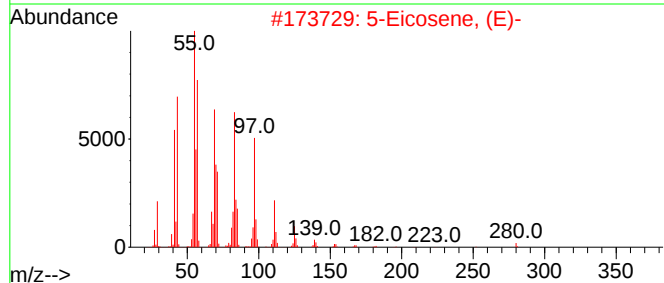
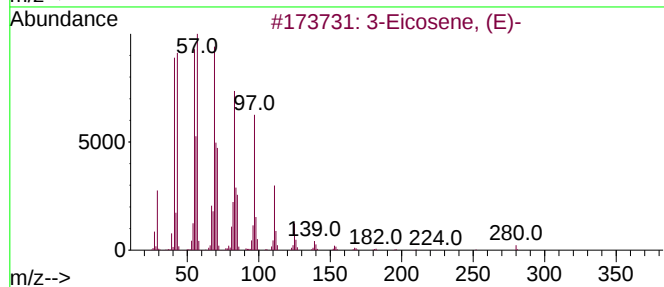
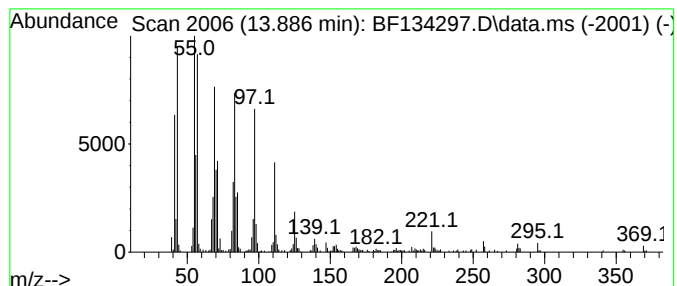
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.886	22.98 ng	659261	Chrysene-d12		14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-		280	C20H40	074685-33-9	98
2	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
3	1-Tetracosene		336	C24H48	010192-32-2	95
4	1-Hexacosene		364	C26H52	018835-33-1	94
5	Behenic alcohol		326	C22H46O	000661-19-8	91



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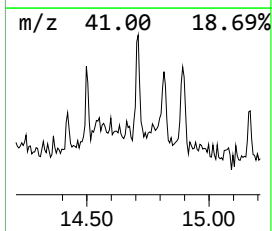
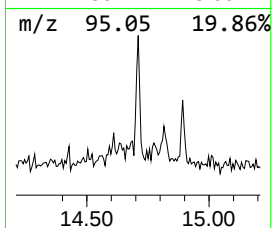
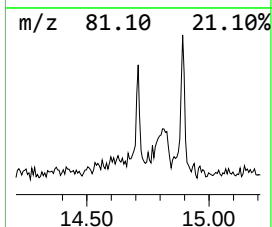
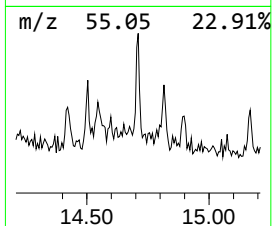
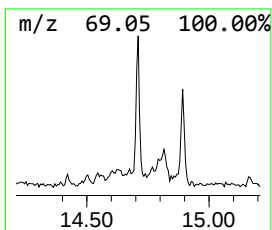
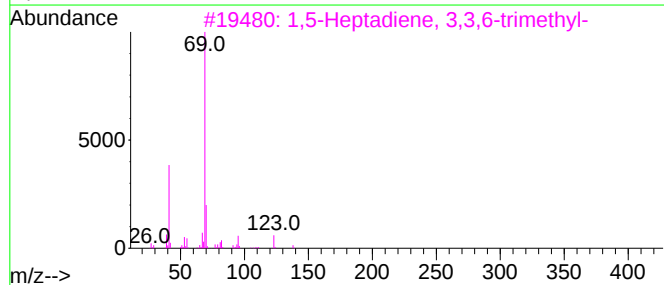
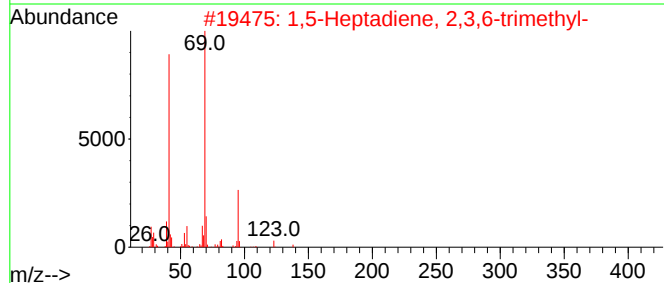
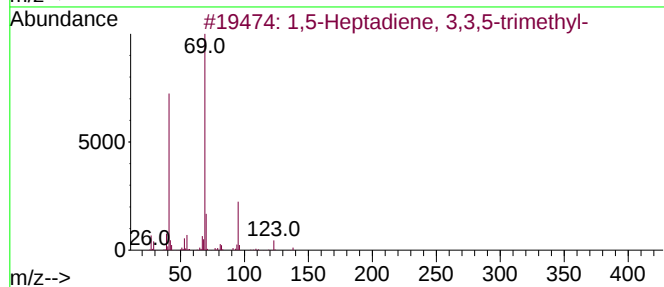
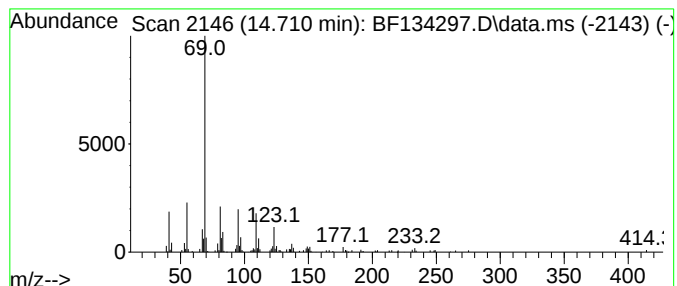
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 1,5-Heptadiene, 3,3,5-trime... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.710	2.92 ng	83784	Chrysene-d12		14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	53
2		1,5-Heptadiene, 2,3,6-trimethyl-	138	C10H18	033501-88-1	50
3		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	47
4		2,6-Dimethyl-2-trans-6-octadiene	138	C10H18	002609-23-6	42
5		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	42



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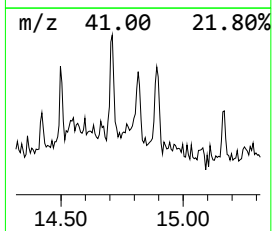
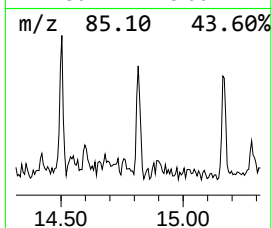
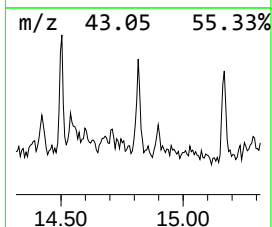
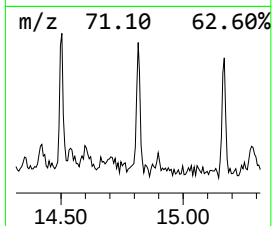
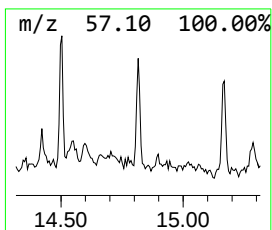
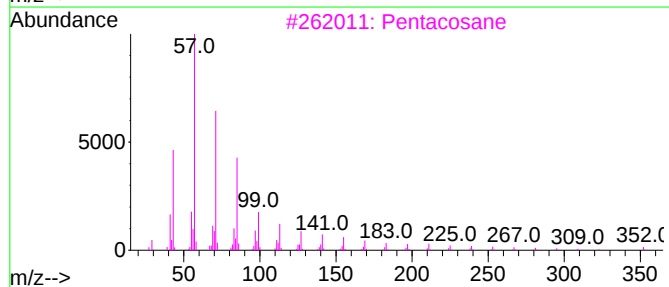
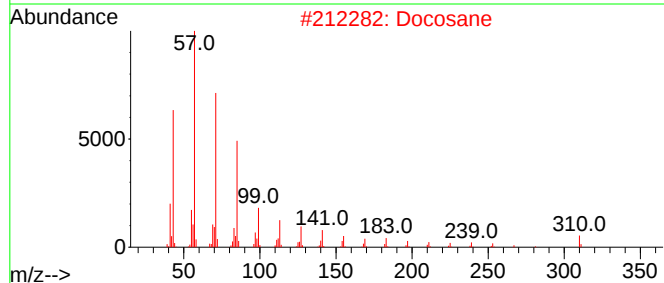
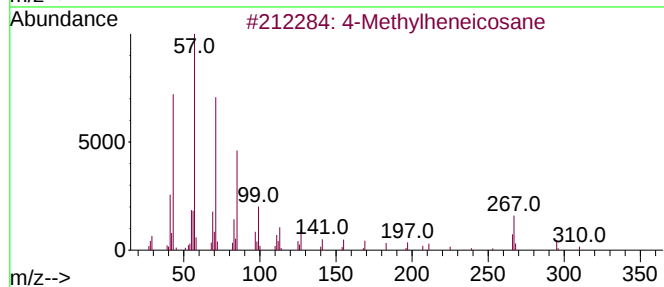
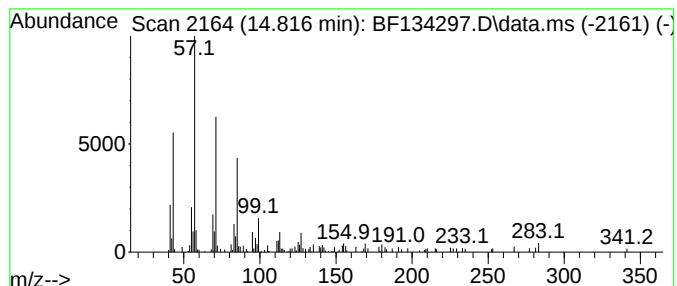
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 4-Methylheneicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	2.96 ng	79443	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methylheneicosane	310	C22H46	025117-29-7	83
2			Docosane	310	C22H46	000629-97-0	83
3			Pentacosane	352	C25H52	000629-99-2	83
4			Hexadecane	226	C16H34	000544-76-3	80
5			Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134297.D
Acq On : 14 Jul 2023 19:02
Operator : CG\JU
Sample : 03563-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HOUSE-BASEMENT

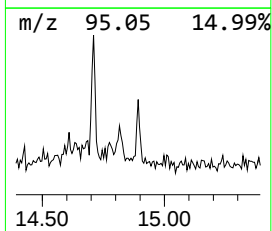
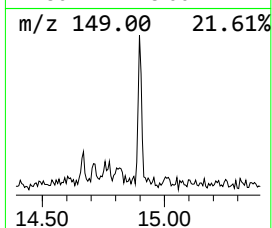
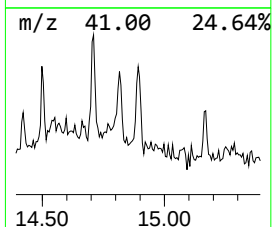
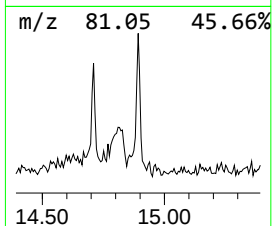
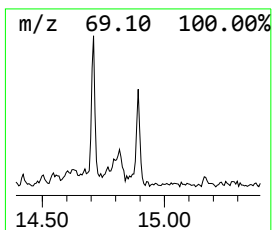
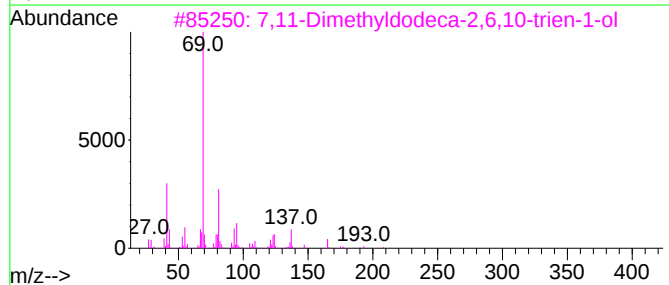
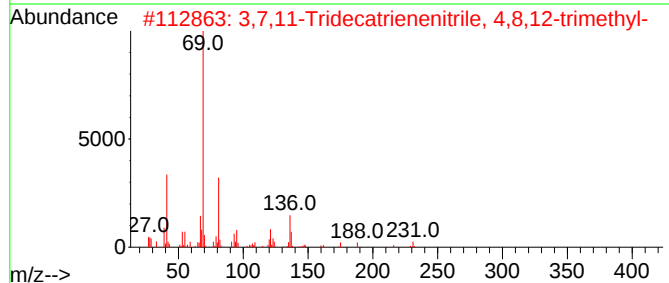
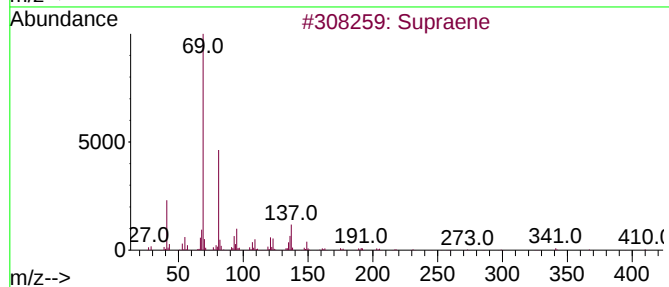
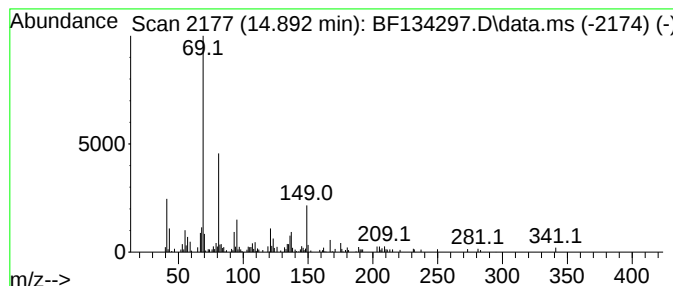
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Supraene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.892	2.67 ng	71702	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	64
2			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	59
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	53
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	53
5			5-Bromo-1-pentanol	166	C5H11BrO	034626-51-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134297.D
Acq On : 14 Jul 2023 19:02
Operator : CG\JU
Sample : 03563-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

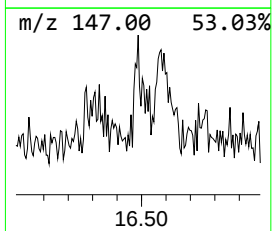
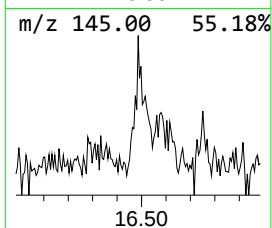
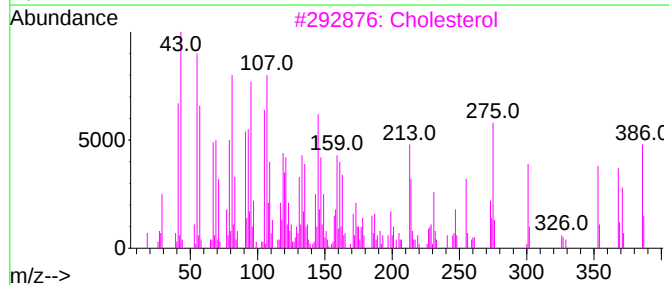
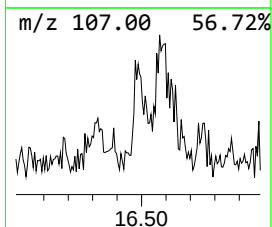
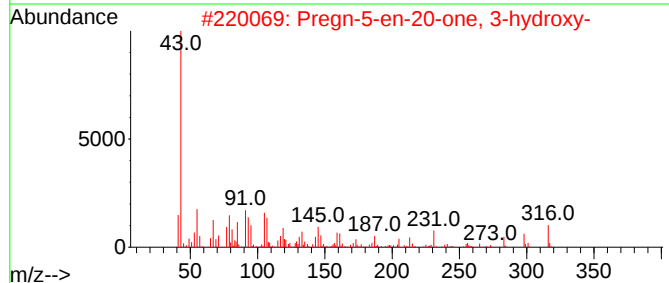
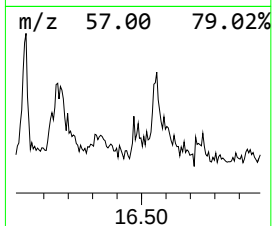
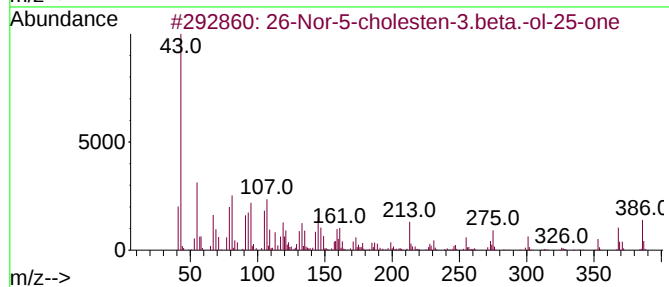
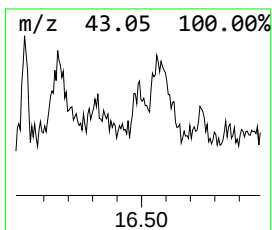
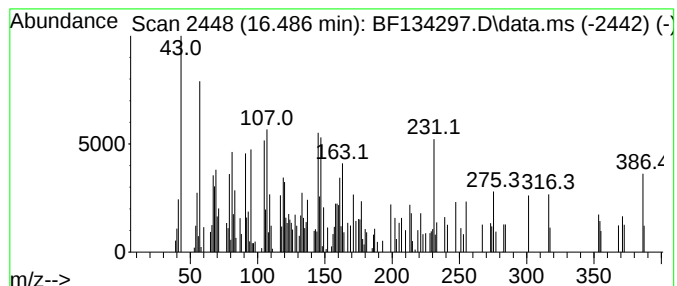
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ClientSampleId :
HOUSE-BASEMENT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 26-Nor-5-cholesten-3.beta.-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.486	5.03 ng	135031	Perylene-d12	15.539	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	64
2	Pregn-5-en-20-one, 3-hydroxy-	316	C21H32O2	038372-24-6	43
3	Cholesterol	386	C27H46O	000057-88-5	41
4	Cholest-5-en-3-ol (3.beta.)-, pr...	442	C30H50O2	000633-31-8	38
5	Cholestan-3-one, (5.beta.)-	386	C27H46O	000601-53-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
Data File : BF134297.D
Acq On : 14 Jul 2023 19:02
Operator : CG\JU
Sample : 03563-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HOUSE-BASEMENT

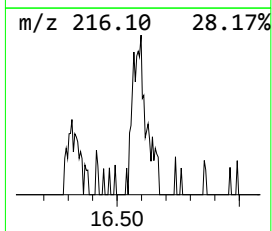
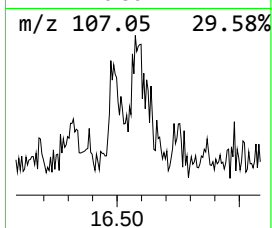
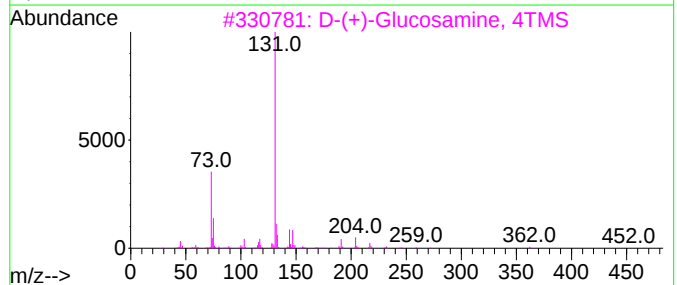
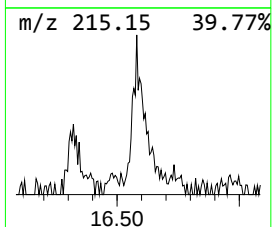
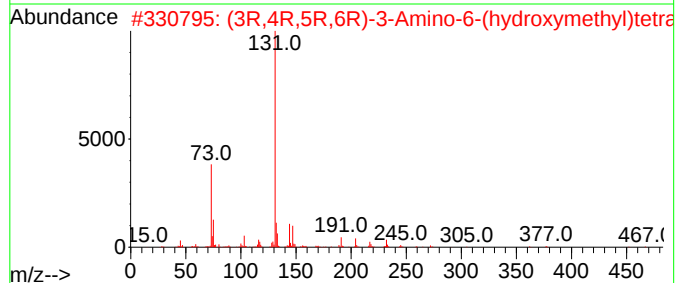
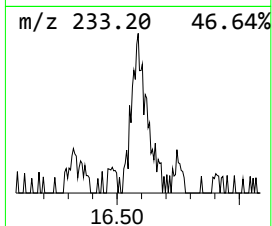
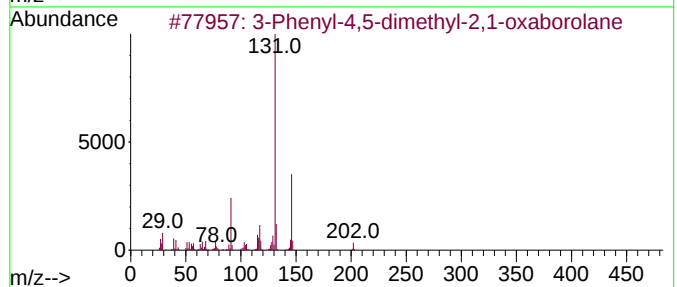
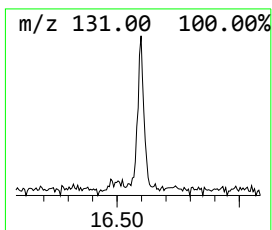
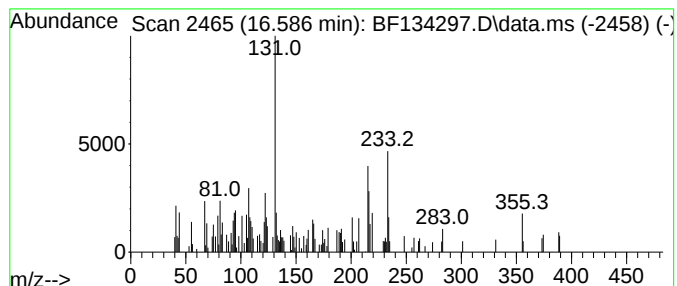
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown16.586 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	8.28 ng	222231	Perylene-d12	15.539

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Phenyl-4,5-dimethyl-2,1-oxabor...	202	C13H19BO	1000062-26-1	18
2		(3R,4R,5R,6R)-3-Amino-6-(hydroxy...	467	C18H45NO5Si4	1000498-23-2	14
3		D-(+)-Glucosamine, 4TMS	467	C18H45NO5Si4	943622-44-4	14
4		(S)-(-)-.alpha.-Terpineol, TMS d...	226	C13H26OSi	057304-99-1	14
5		1.6-Farnesadiene-3.10.11-triol, ...	472	C24H52O3Si3	1000512-91-4	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
 Data File : BF134297.D
 Acq On : 14 Jul 2023 19:02
 Operator : CG\JU
 Sample : 03563-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HOUSE-BASEMENT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
Benzenemethanam...	7.034	4.3	ng	101307	1	6.840	474463	20.0
Cyclohexanol, 2...	8.028	3.4	ng	119745	2	8.122	705367	20.0
unknown8.240	8.240	9.6	ng	338410	2	8.122	705367	20.0
Cyclohexanol, 4...	8.292	2.9	ng	101495	2	8.122	705367	20.0
4,7-Methano-1H-...	8.716	18.4	ng	647847	2	8.122	705367	20.0
Indole	8.763	3.6	ng	125480	2	8.122	705367	20.0
Benzophenone	10.598	9.3	ng	392737	3	9.881	843339	20.0
Amberonne (isom...	10.739	2.8	ng	102550	4	11.375	721528	20.0
Dimethyl palmit...	10.810	4.7	ng	168176	4	11.375	721528	20.0
7-Acetyl-6-ethy...	11.545	4.6	ng	165686	4	11.375	721528	20.0
cis-7-Hexadecen...	11.839	5.9	ng	212280	4	11.375	721528	20.0
n-Hexadecanoic ...	11.916	31.8	ng	1146710	4	11.375	721528	20.0
Octadecanoic acid	12.698	8.9	ng	321848	4	11.375	721528	20.0
Ethanol, 2-buto...	13.533	3.3	ng	93747	5	14.033	573779	20.0
3-Eicosene, (E)-	13.886	23.0	ng	659261	5	14.033	573779	20.0
1,5-Heptadiene,...	14.710	2.9	ng	83784	5	14.033	573779	20.0
4-Methylheneico...	14.816	3.0	ng	79443	6	15.539	536706	20.0
Supraene	14.892	2.7	ng	71702	6	15.539	536706	20.0
26-Nor-5-choles...	16.486	5.0	ng	135031	6	15.539	536706	20.0
unknown16.586	16.586	8.3	ng	222231	6	15.539	536706	20.0