

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
 Data File : BF135024.D
 Acq On : 31 Aug 2023 01:53
 Operator : CG\JU
 Sample : 04196-29
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-345-COMP-05

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-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135024.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	17	rBV	38136	53654	2.18%	0.246%
2	5.004	492	496	504	rVB	80964	101324	4.12%	0.465%
3	5.404	559	564	567	rBV	2534664	2428401	98.64%	11.150%
4	6.410	730	735	738	rBV	2555898	2402294	97.58%	11.030%
5	6.604	764	768	779	rBV	139844	136178	5.53%	0.625%
6	6.769	793	796	800	rBV	975690	775996	31.52%	3.563%
7	7.334	887	892	895	rBV	1736793	1494956	60.72%	6.864%
8	8.051	1010	1014	1017	rBV	1215463	996065	40.46%	4.574%
9	9.128	1193	1197	1200	rBV	2833745	2461879	100.00%	11.304%
10	9.251	1213	1218	1222	rBV	1505084	1495447	60.74%	6.866%
11	9.669	1286	1289	1292	rBV	31920	27188	1.10%	0.125%
12	9.810	1309	1313	1316	rVB	1140927	1001273	40.67%	4.597%
13	10.598	1443	1447	1450	rBV	1580198	1307052	53.09%	6.001%
14	10.886	1492	1496	1502	rBV	33882	43744	1.78%	0.201%
15	11.298	1562	1566	1569	rBV	986250	858556	34.87%	3.942%
16	11.322	1569	1570	1573	rVV	230715	154641	6.28%	0.710%
17	11.375	1576	1579	1582	rVB	33695	28507	1.16%	0.131%
18	11.704	1628	1635	1641	rVB3	38233	43696	1.77%	0.201%
19	11.804	1649	1652	1654	rBV	54311	44302	1.80%	0.203%
20	11.839	1654	1658	1663	rVV2	254078	264503	10.74%	1.214%
21	11.916	1668	1671	1673	rVV	71007	70987	2.88%	0.326%
22	11.939	1673	1675	1680	rVB	43041	34914	1.42%	0.160%
23	12.104	1697	1703	1705	rBV2	30388	30852	1.25%	0.142%
24	12.127	1705	1707	1710	rVB2	38587	32876	1.34%	0.151%
25	12.357	1743	1746	1749	rBV	43958	48365	1.96%	0.222%
26	12.392	1749	1752	1754	rVV2	42960	48702	1.98%	0.224%
27	12.416	1754	1756	1758	rVV	134199	101140	4.11%	0.464%
28	12.439	1758	1760	1765	rVB2	32883	35670	1.45%	0.164%
29	12.516	1768	1773	1777	rBV	279456	275059	11.17%	1.263%
30	12.563	1777	1781	1784	rBV2	30883	36701	1.49%	0.169%
31	12.627	1788	1792	1798	rBV3	62150	90798	3.69%	0.417%
32	12.745	1806	1812	1815	rBV	258362	271351	11.02%	1.246%
33	12.898	1834	1838	1841	rBV	1758811	1500135	60.93%	6.888%
34	12.969	1845	1850	1853	rBV3	31725	46246	1.88%	0.212%
35	13.080	1866	1869	1872	rVB	39920	40095	1.63%	0.184%
36	13.145	1873	1880	1883	rBV3	34691	47563	1.93%	0.218%

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Peak Location: TOP

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37	13.180	1883	1886	1891	rVV2	38384	43212	1.76%	0.198%
38	13.486	1934	1938	1944	rVB4	22880	34933	1.42%	0.160%
39	13.592	1953	1956	1961	rVB	32366	39060	1.59%	0.179%
40	13.704	1970	1975	1978	rBV3	40211	59162	2.40%	0.272%
41	13.810	1989	1993	2000	rBV3	92634	140380	5.70%	0.645%
42	13.957	2011	2018	2020	rBV2	727803	815424	33.12%	3.744%
43	13.980	2020	2022	2025	rVB	137663	111540	4.53%	0.512%
44	14.345	2081	2084	2088	rVB	60899	55255	2.24%	0.254%
45	14.380	2088	2090	2093	rVB2	35028	30174	1.23%	0.139%
46	14.468	2103	2105	2112	rVB3	32535	49689	2.02%	0.228%
47	14.821	2161	2165	2172	rBV2	65002	81519	3.31%	0.374%
48	14.898	2174	2178	2183	rVB3	34834	47575	1.93%	0.218%
49	14.998	2190	2195	2206	rBV	137185	262721	10.67%	1.206%
50	15.098	2208	2212	2215	rBV2	27025	45076	1.83%	0.207%
51	15.298	2242	2246	2252	rVB	84057	108755	4.42%	0.499%
52	15.357	2252	2256	2262	rBV	105495	132867	5.40%	0.610%
53	15.421	2262	2267	2272	rBV	552095	701858	28.51%	3.223%
54	15.915	2347	2351	2358	rBV2	34036	56771	2.31%	0.261%
55	16.898	2512	2518	2525	rBV3	37736	83255	3.38%	0.382%
56	17.339	2590	2593	2601	rVB2	27730	48607	1.97%	0.223%

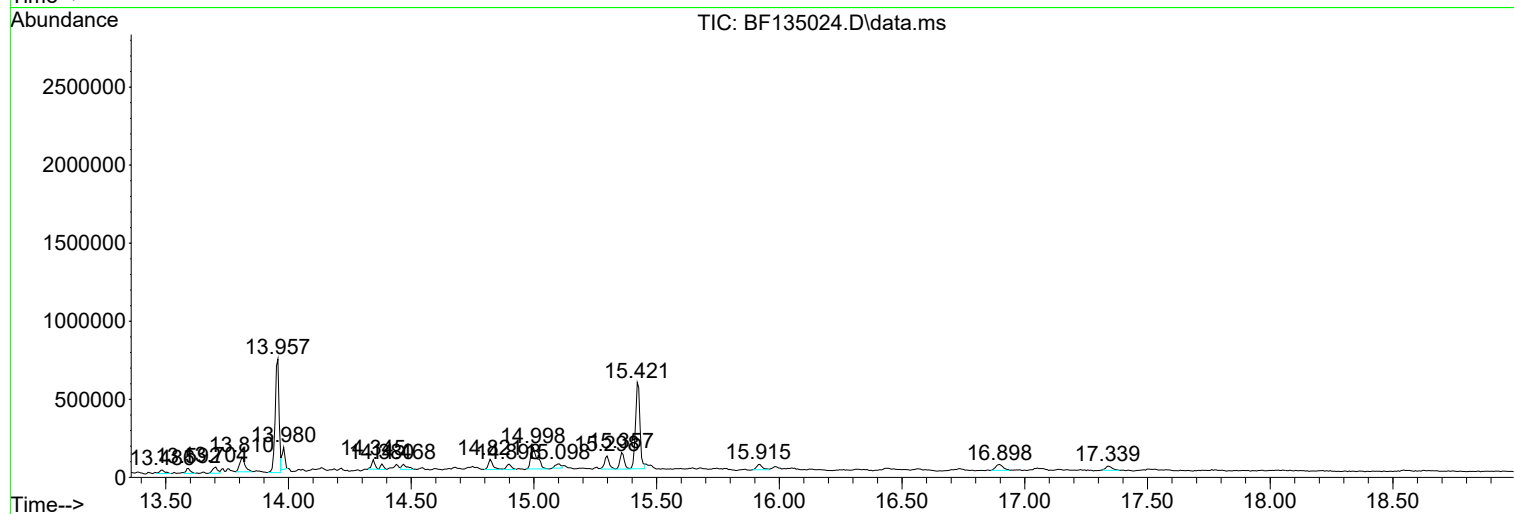
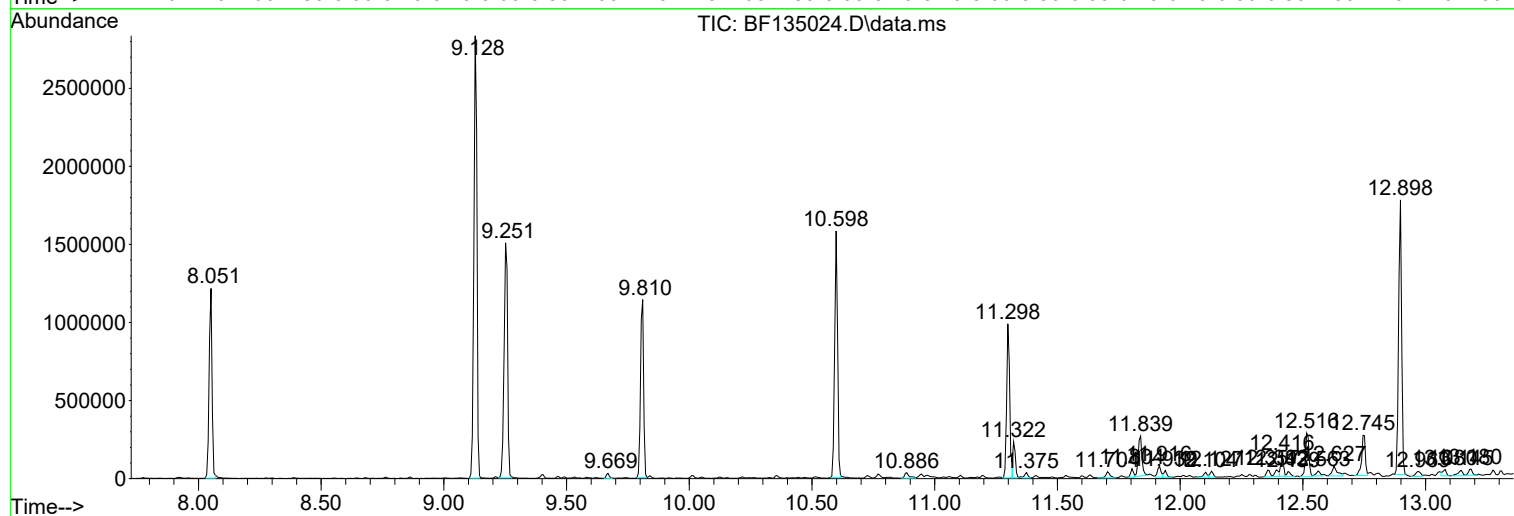
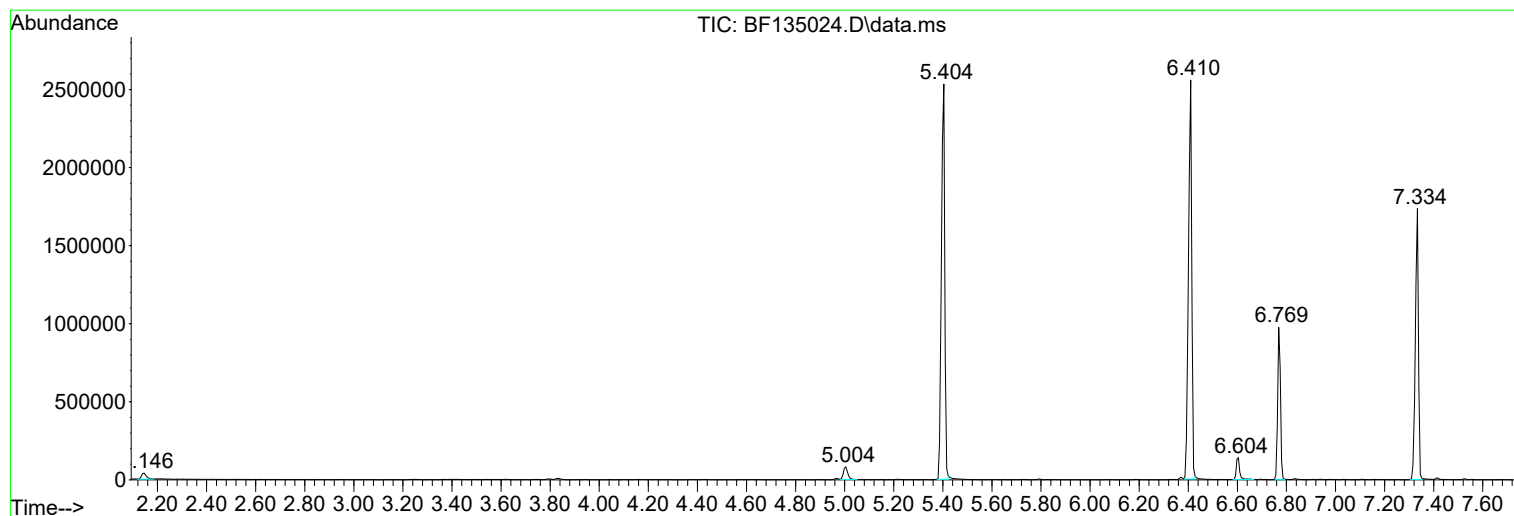
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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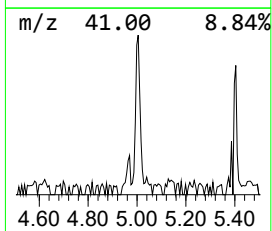
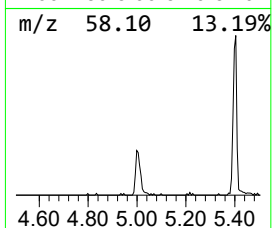
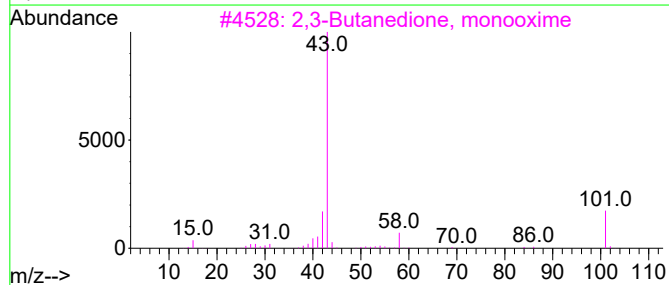
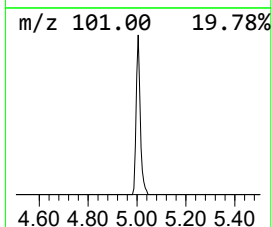
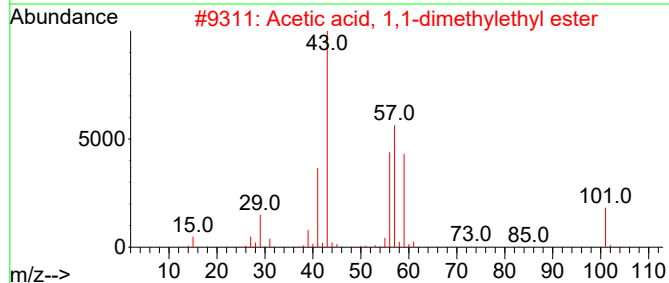
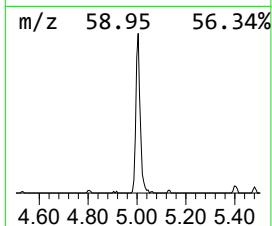
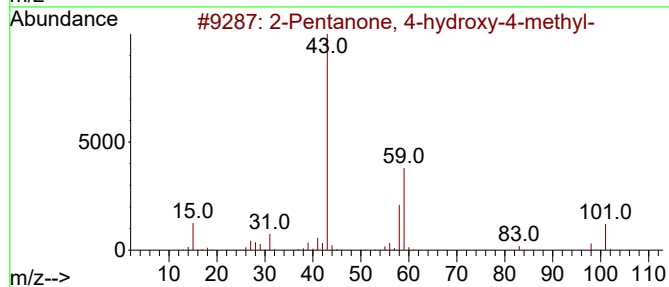
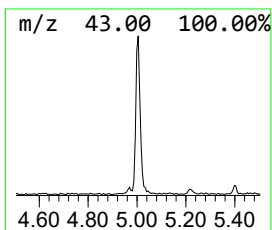
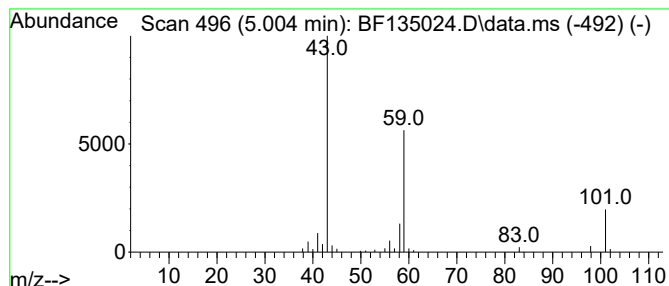
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.61 ng	101324	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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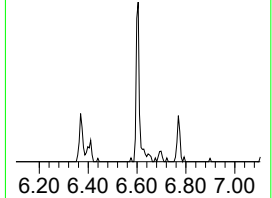
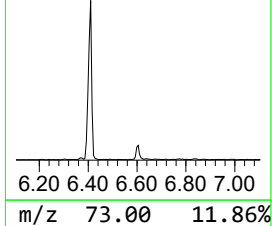
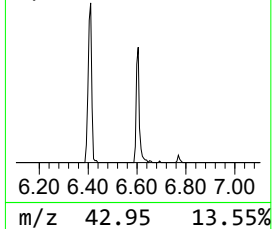
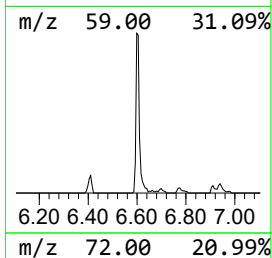
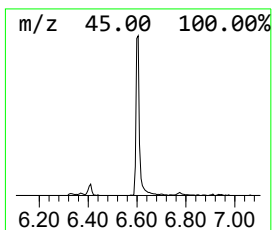
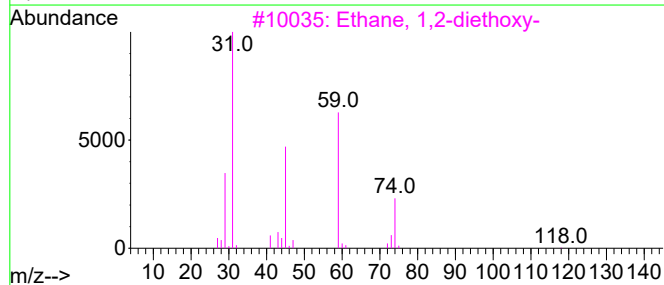
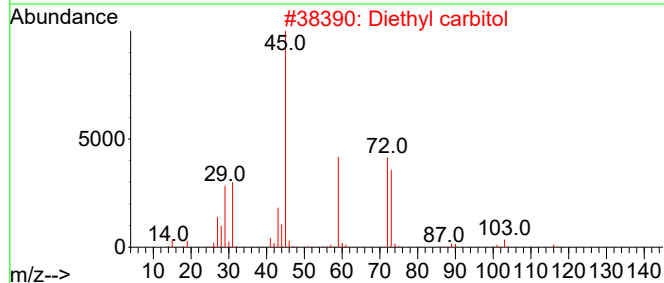
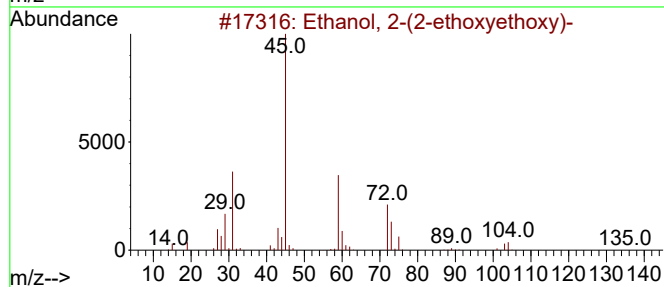
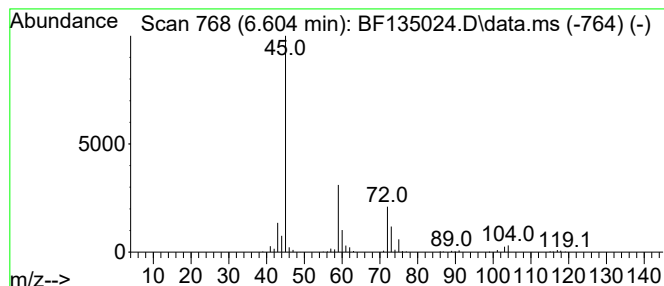
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	3.51 ng	136178	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	50
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42



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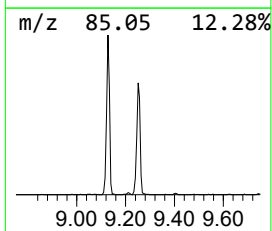
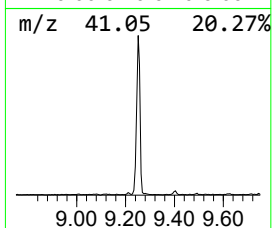
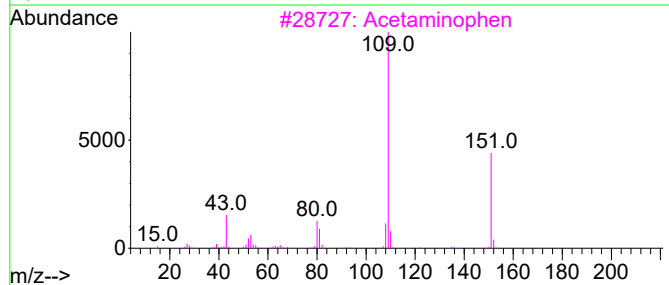
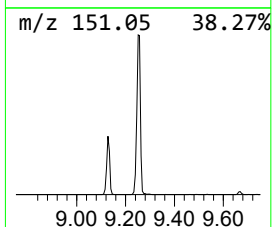
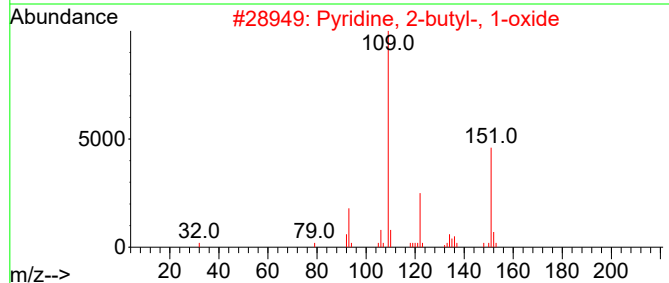
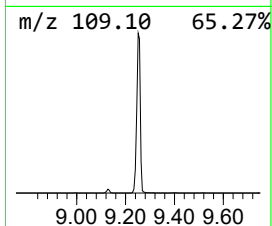
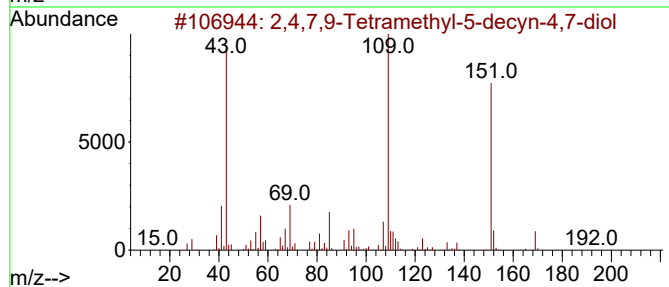
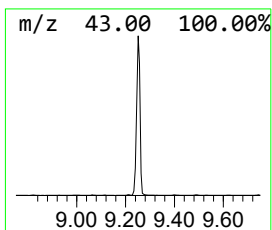
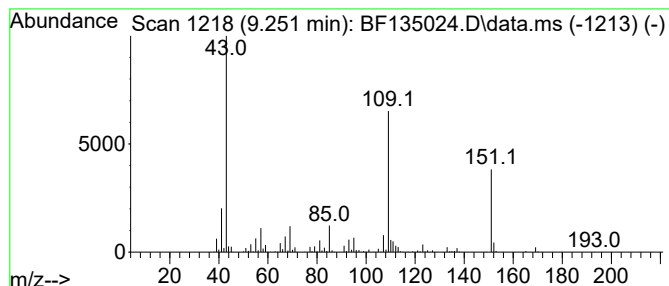
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.251	29.87 ng	1495450	Acenaphthene-d10		9.810	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	59
3	Acetaminophen		151	C8H9NO2	000103-90-2	58
4	Metacetamol		151	C8H9NO2	000621-42-1	53
5	benzenamine, 3-[(tetrahydro-2H-p...		193	C11H15NO2	1010400-28-1	27



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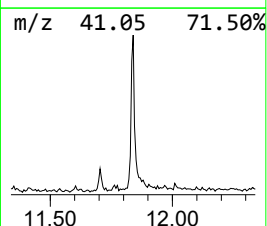
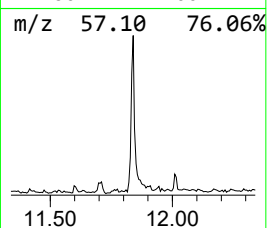
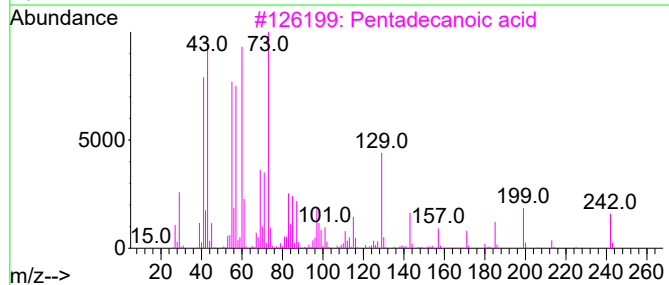
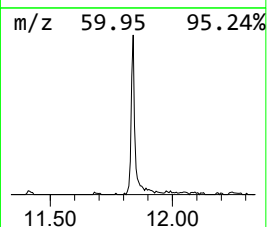
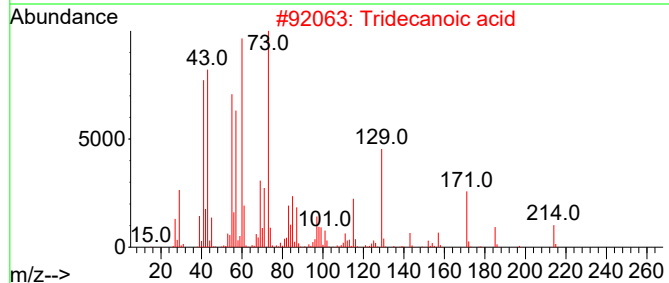
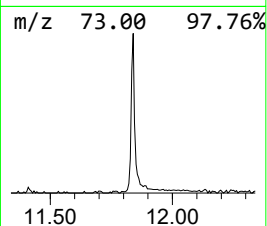
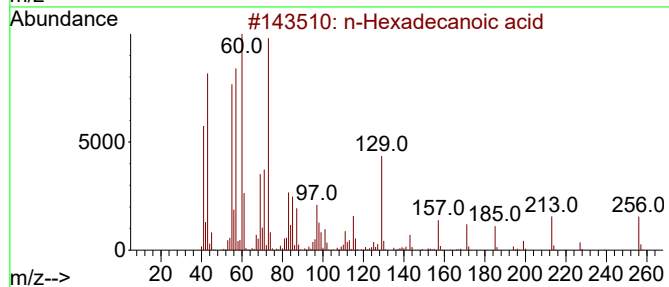
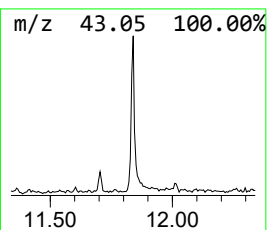
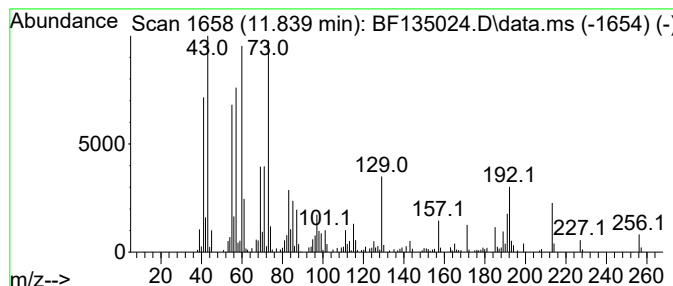
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	6.16 ng	264503	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	74



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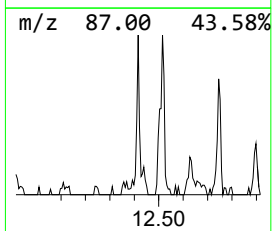
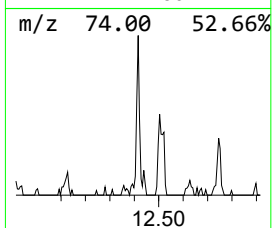
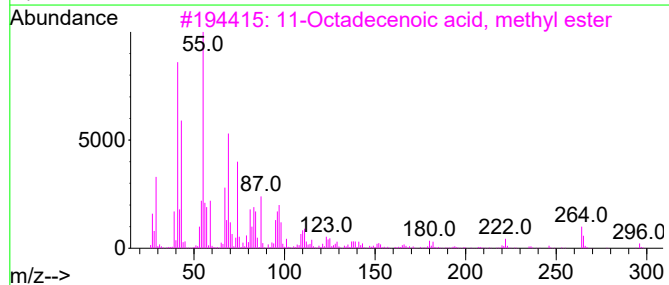
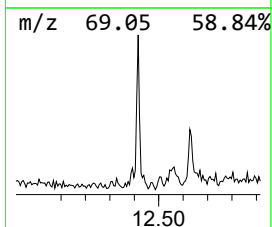
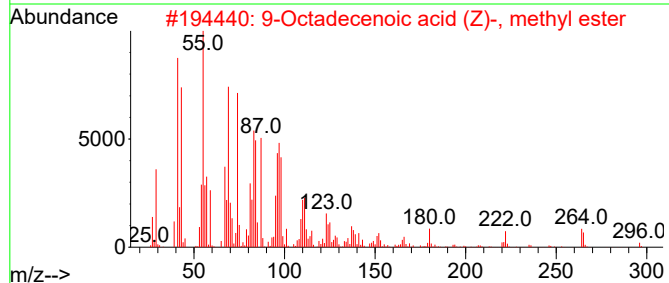
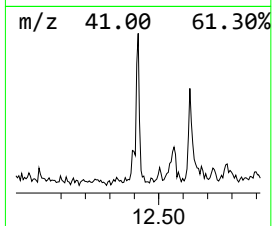
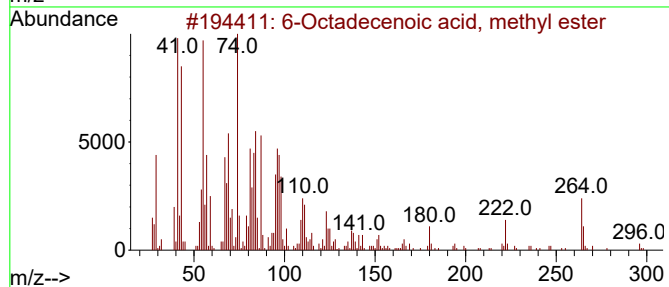
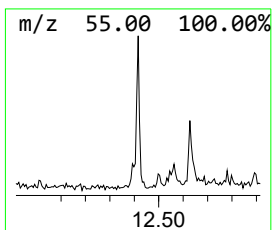
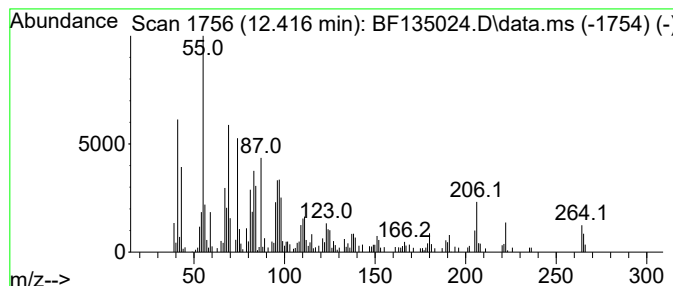
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 6-Octadecenoic acid, methyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	2.36 ng	101140	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	93
2			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
3			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	90
4			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	90
5			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135024.D
Acq On : 31 Aug 2023 01:53
Operator : CG\JU
Sample : 04196-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-05

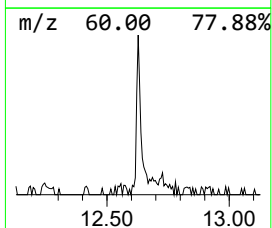
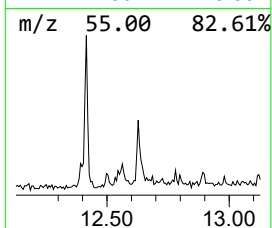
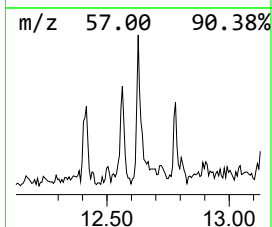
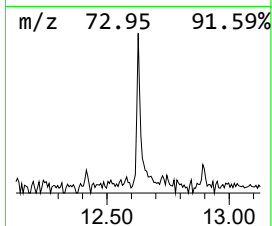
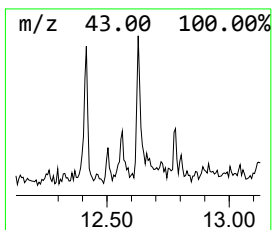
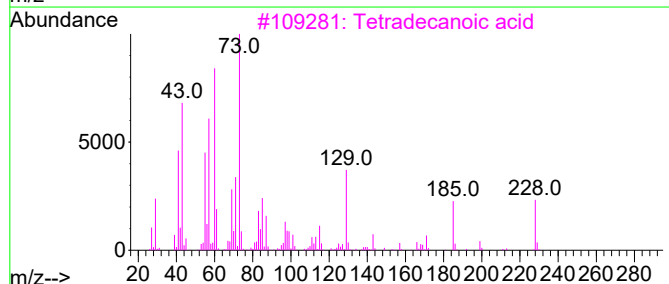
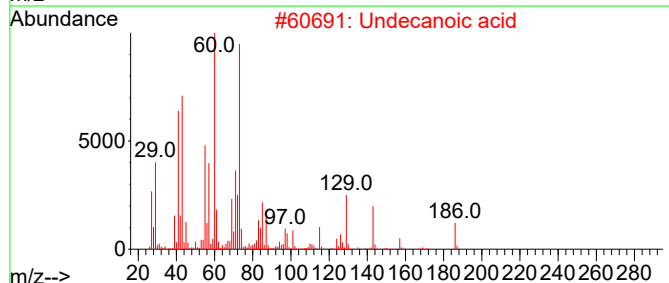
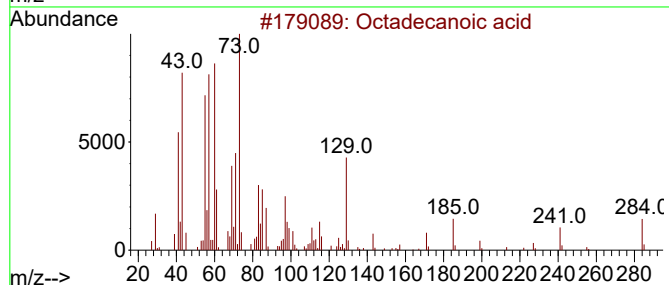
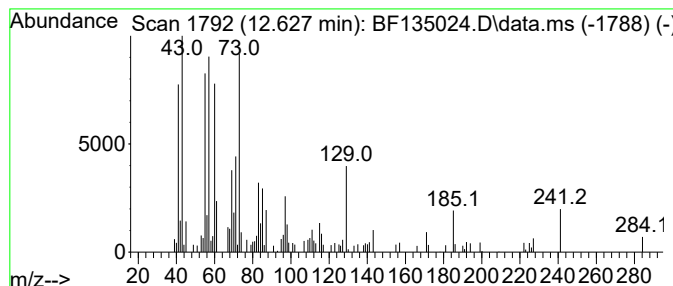
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	2.23 ng	90798	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	87
2			Undecanoic acid	186	C11H22O2	000112-37-8	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135024.D
Acq On : 31 Aug 2023 01:53
Operator : CG\JU
Sample : 04196-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-05

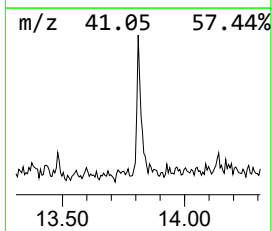
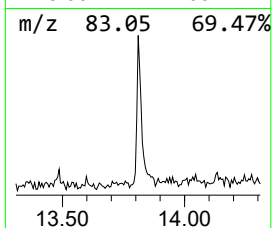
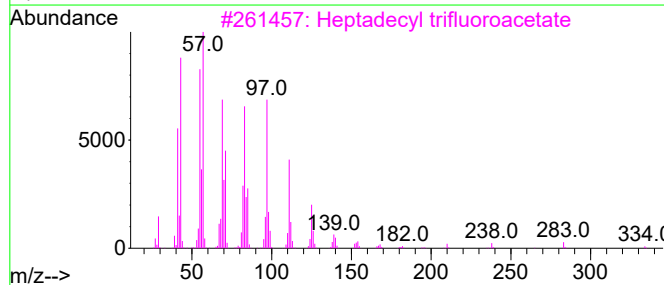
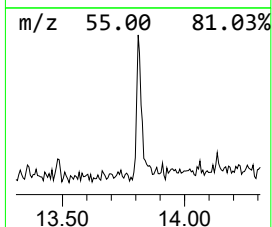
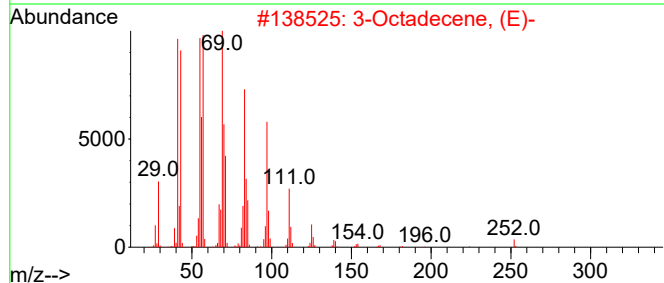
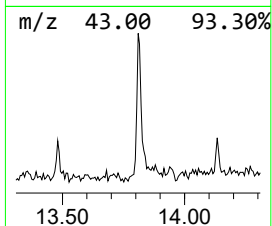
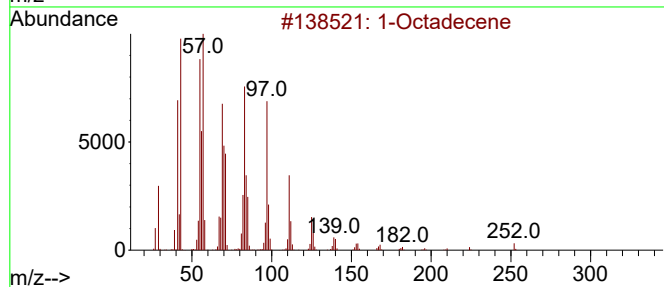
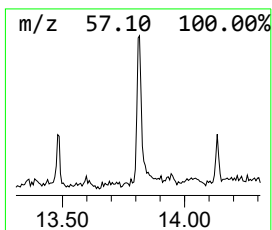
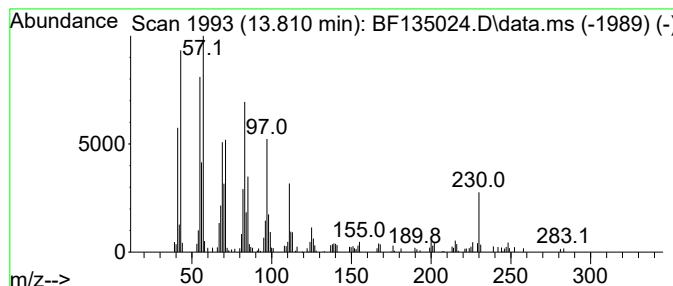
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	3.44 ng	140380	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	92
2			3-Octadecene, (E)-	252	C18H36	007206-19-1	87
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	87
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135024.D
Acq On : 31 Aug 2023 01:53
Operator : CG\JU
Sample : 04196-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-05

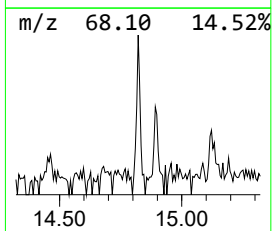
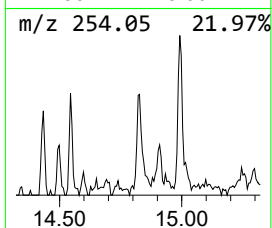
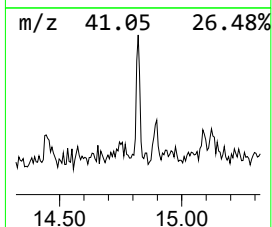
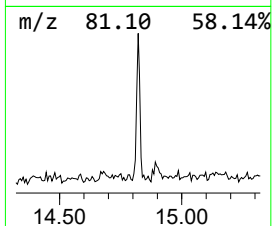
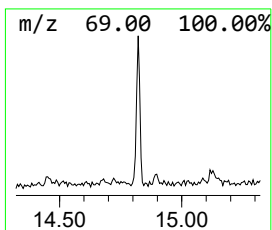
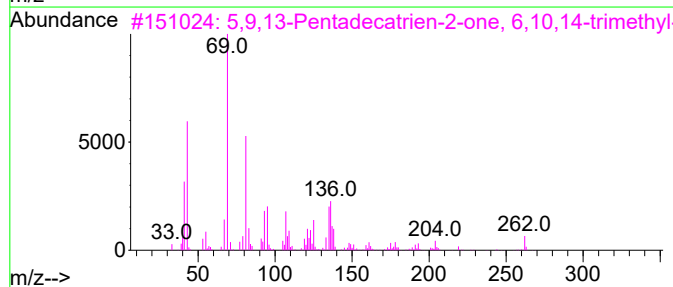
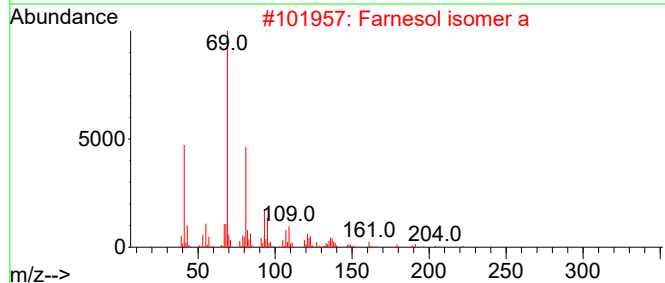
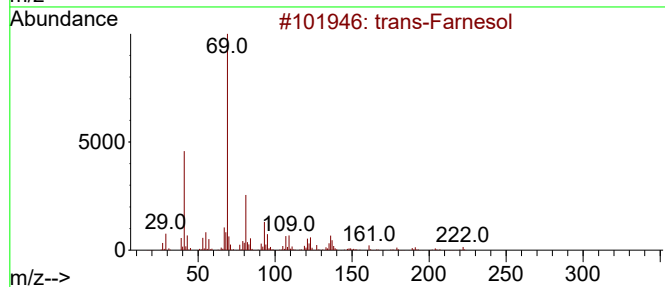
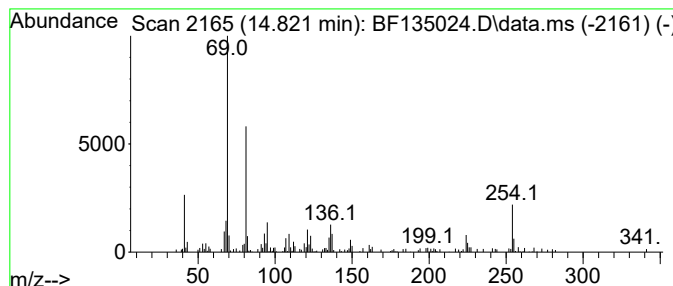
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 trans-Farnesol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	2.32 ng	81519	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Farnesol	222	C15H26O	000106-28-5	76
2			Farnesol isomer a	222	C15H26O	1000108-92-4	70
3			5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	000762-29-8	53
4			2-propenamide, 2-methyl-N-[4-(m...	254	C11H14N2O3S	1000401-43-5	50
5			.beta.-Citronellol, chlorodifluo...	268	C12H19ClF2O2	1000376-20-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135024.D
Acq On : 31 Aug 2023 01:53
Operator : CG\JU
Sample : 04196-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
OR-345-COMP-05

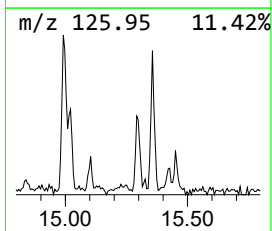
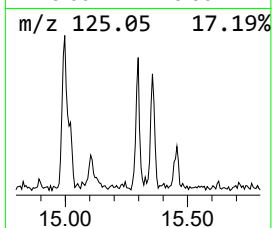
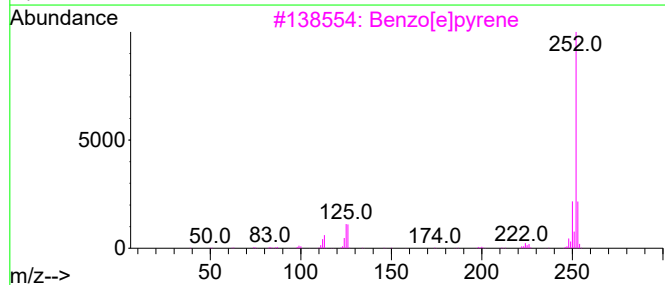
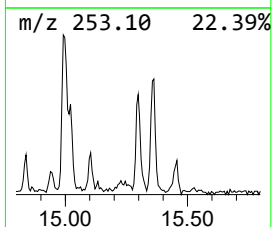
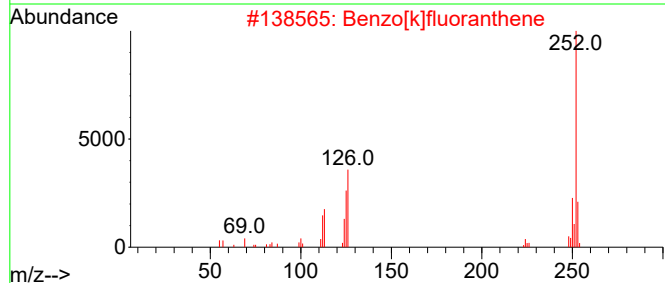
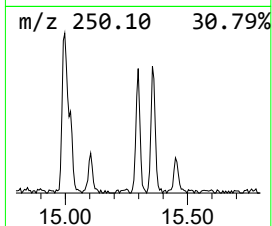
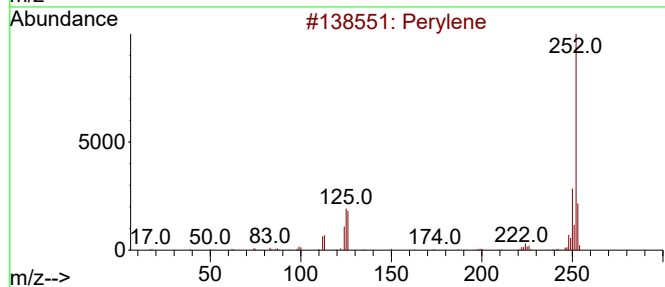
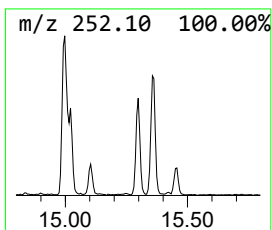
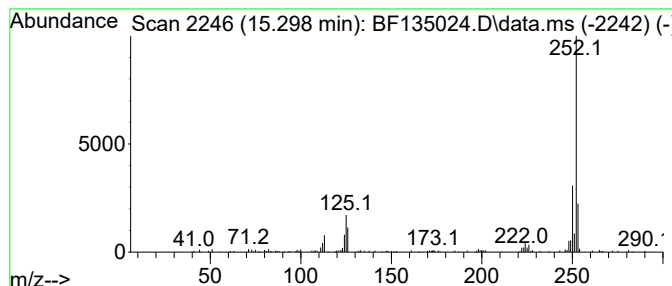
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	3.10 ng	108755	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	95
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3			Benzo[e]pyrene	252	C20H12	000192-97-2	93
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	91
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135024.D
Acq On : 31 Aug 2023 01:53
Operator : CG\JU
Sample : 04196-29
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-05

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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
2-Pentanone, 4-...	5.004	2.6	ng	101324	1	6.769	775996	20.0
Ethanol, 2-(2-e...	6.604	3.5	ng	136178	1	6.769	775996	20.0
2,4,7,9-Tetrame...	9.251	29.9	ng	1495450	3	9.810	1001270	20.0
n-Hexadecanoic ...	11.839	6.2	ng	264503	4	11.298	858556	20.0
6-Octadecenoic ...	12.416	2.4	ng	101140	4	11.298	858556	20.0
Octadecanoic acid	12.627	2.2	ng	90798	5	13.957	815424	20.0
1-Octadecene	13.810	3.4	ng	140380	5	13.957	815424	20.0
trans-Farnesol	14.821	2.3	ng	81519	6	15.421	701858	20.0
Perylene	15.298	3.1	ng	108755	6	15.421	701858	20.0