

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060525\
 Data File : BF142635.D
 Acq On : 05 Jun 2025 15:36
 Operator : RC/JU
 Sample : Q2199-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11978

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-BF052025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	487	496	507	rBV	155076	225776	10.23%	1.033%
2	5.510	558	564	570	rBV	1457325	1980350	89.70%	9.063%
3	6.522	730	736	741	rBV	1396294	1896693	85.91%	8.680%
4	6.598	745	749	755	rVB	18573	23987	1.09%	0.110%
5	6.892	794	799	805	rBV	590041	724961	32.84%	3.318%
6	7.457	889	895	900	rBV	947067	1224297	55.46%	5.603%
7	8.181	1012	1018	1035	rVB	670987	879228	39.83%	4.024%
8	9.251	1195	1200	1205	rBV	1789346	2207665	100.00%	10.103%
9	9.933	1311	1316	1320	rBV	650757	800812	36.27%	3.665%
10	10.480	1405	1409	1415	rVB	29359	38423	1.74%	0.176%
11	10.575	1415	1425	1431	rBV8	8512	28791	1.30%	0.132%
12	10.645	1432	1437	1444	rVV	293997	367188	16.63%	1.680%
13	10.722	1445	1450	1461	rVV	820354	1050022	47.56%	4.805%
14	10.839	1465	1470	1476	rVB4	21363	39100	1.77%	0.179%
15	10.957	1486	1490	1496	rVB	49173	62126	2.81%	0.284%
16	11.422	1564	1569	1578	rBV2	523968	837162	37.92%	3.831%
17	11.498	1578	1582	1585	rVB	31078	39079	1.77%	0.179%
18	11.645	1601	1607	1615	rBV3	28531	62448	2.83%	0.286%
19	11.945	1650	1658	1664	rBV2	140073	252423	11.43%	1.155%
20	12.033	1670	1673	1681	rVB	52044	90473	4.10%	0.414%
21	12.110	1681	1686	1691	rBV6	14087	33337	1.51%	0.153%
22	12.198	1697	1701	1703	rBV3	22537	33353	1.51%	0.153%
23	12.369	1724	1730	1732	rBV5	16433	25115	1.14%	0.115%
24	12.504	1750	1753	1759	rVB5	20743	34971	1.58%	0.160%
25	12.557	1759	1762	1767	rVB3	22701	31735	1.44%	0.145%
26	12.633	1770	1775	1779	rBV	278782	362518	16.42%	1.659%
27	12.669	1779	1781	1788	rVB7	15499	23100	1.05%	0.106%
28	12.727	1788	1791	1795	rBV	29502	38493	1.74%	0.176%
29	12.863	1808	1814	1821	rBV	235559	357861	16.21%	1.638%
30	13.004	1831	1838	1846	rBV	1366670	1879819	85.15%	8.603%
31	13.086	1847	1852	1859	rBV3	38090	72608	3.29%	0.332%
32	13.186	1862	1869	1873	rBV2	55098	115464	5.23%	0.528%
33	13.257	1878	1881	1884	rVV	33445	42553	1.93%	0.195%
34	13.298	1884	1888	1895	rVB3	45312	88029	3.99%	0.403%
35	13.392	1900	1904	1906	rBV	38013	49382	2.24%	0.226%
36	13.421	1906	1909	1912	rVB2	23867	27818	1.26%	0.127%

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11978

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-BF052025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.698	1954	1956	1961	rVB	36868	48222	2.18%	0.221%
38	13.816	1971	1976	1978	rBV3	41384	71310	3.23%	0.326%
39	13.904	1987	1991	1998	rVB3	101170	168011	7.61%	0.769%
40	14.063	2010	2018	2030	rBV2	751582	1488669	67.43%	6.813%
41	14.451	2080	2084	2087	rBV	56282	74801	3.39%	0.342%
42	14.480	2087	2089	2093	rVB3	35366	40907	1.85%	0.187%
43	14.533	2094	2098	2102	rBV5	64590	123702	5.60%	0.566%
44	14.692	2122	2125	2130	rVB2	57029	75073	3.40%	0.344%
45	15.115	2192	2197	2206	rBV	419393	930226	42.14%	4.257%
46	15.186	2206	2209	2212	rBV2	47525	67993	3.08%	0.311%
47	15.427	2245	2250	2256	rVB	221154	354031	16.04%	1.620%
48	15.492	2256	2261	2267	rVB	211446	311214	14.10%	1.424%
49	15.557	2267	2272	2286	rBV2	496257	956939	43.35%	4.379%
50	16.027	2347	2352	2358	rBV	81854	143823	6.51%	0.658%
51	16.857	2487	2493	2507	rBV6	51599	149772	6.78%	0.685%
52	17.062	2523	2528	2535	rBV2	73503	155873	7.06%	0.713%
53	17.251	2555	2560	2565	rBV4	35261	79044	3.58%	0.362%
54	17.421	2584	2589	2598	rVB2	89543	203145	9.20%	0.930%
55	17.515	2600	2605	2618	rVB	66738	162981	7.38%	0.746%
56	17.674	2625	2632	2643	rBV8	56538	198335	8.98%	0.908%

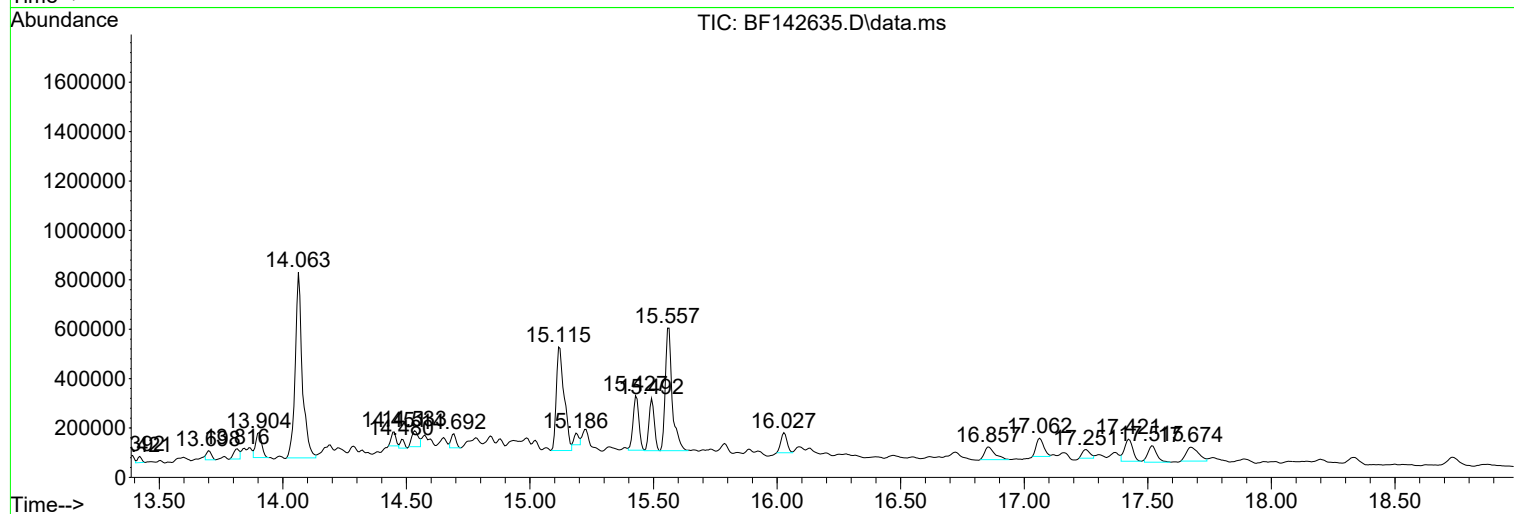
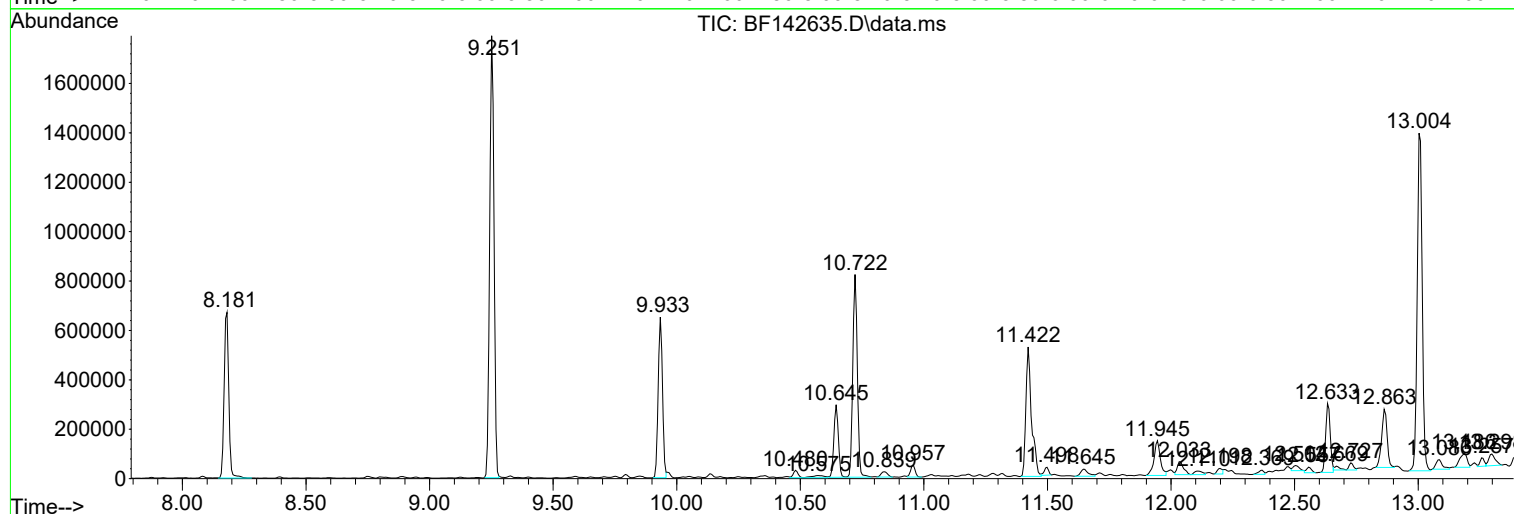
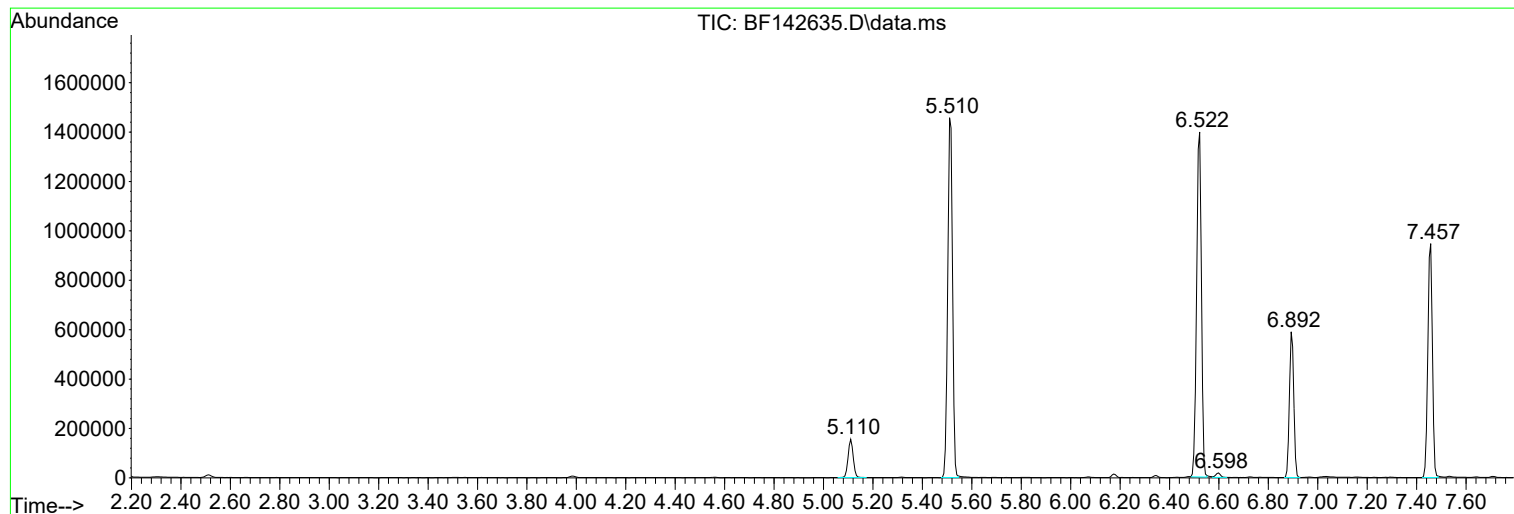
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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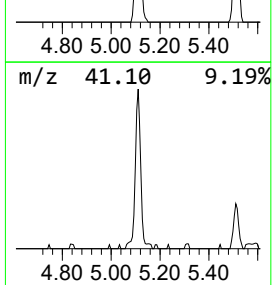
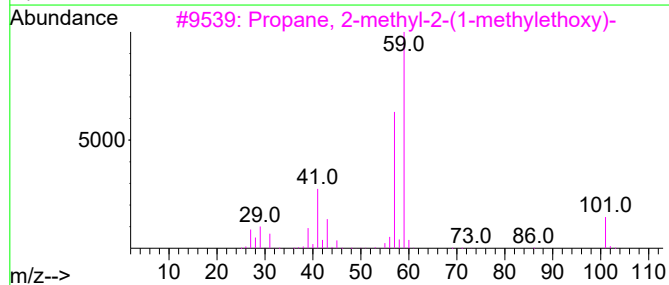
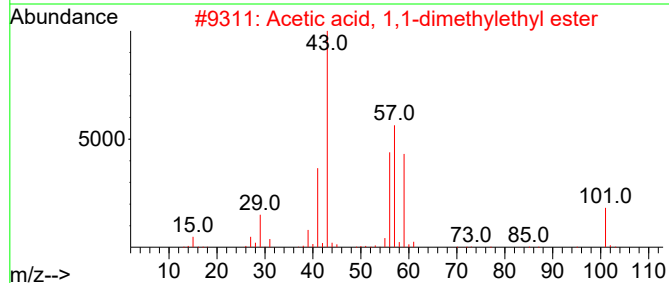
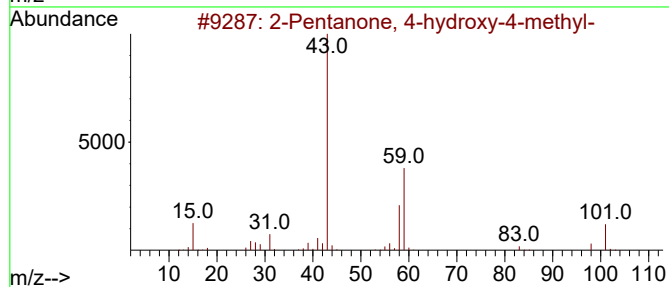
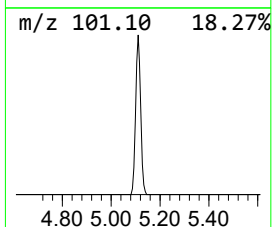
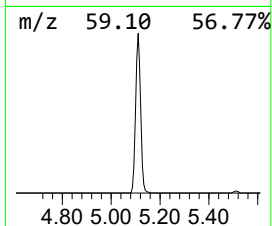
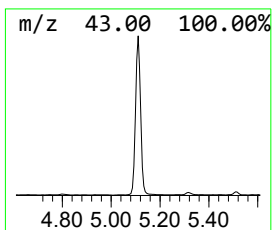
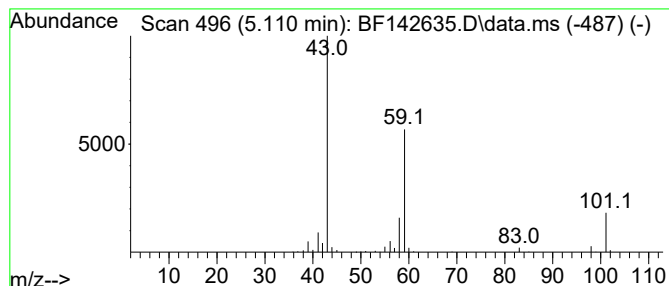
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	6.23 ng	225776	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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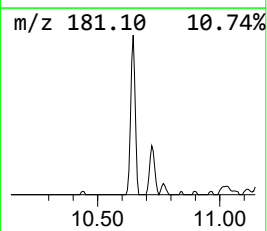
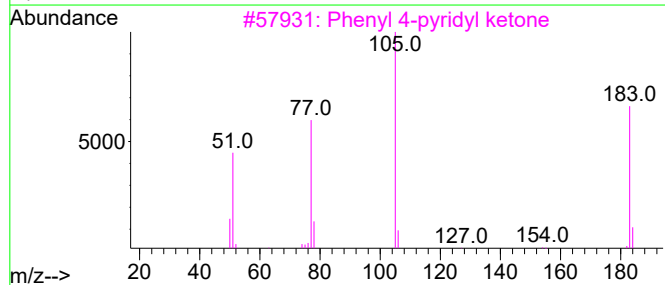
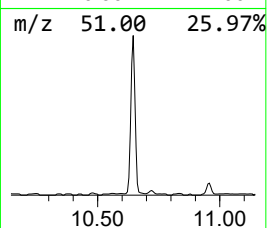
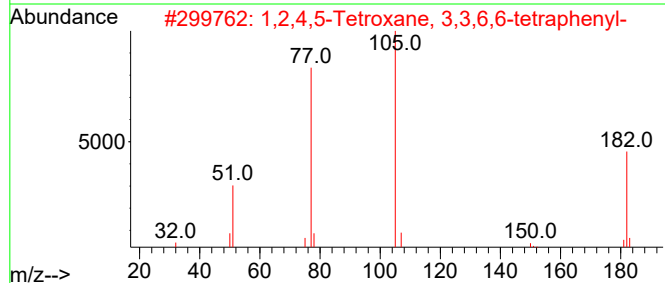
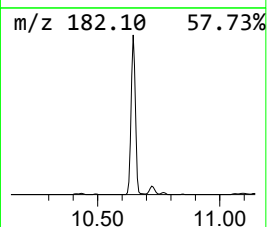
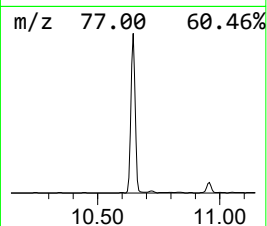
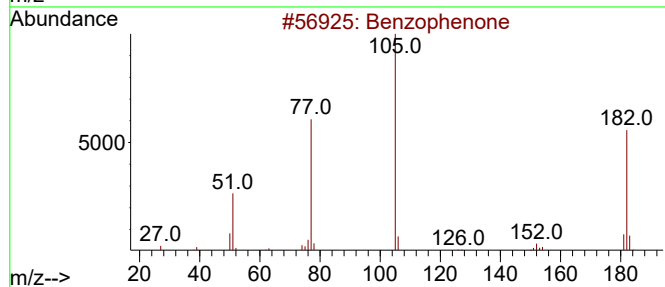
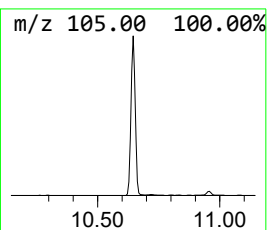
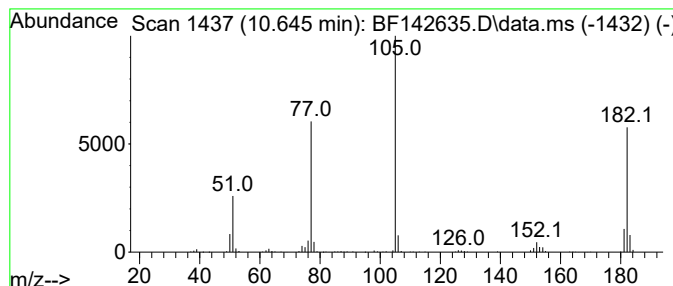
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.645	9.17 ng	367188	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47



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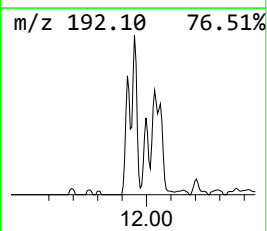
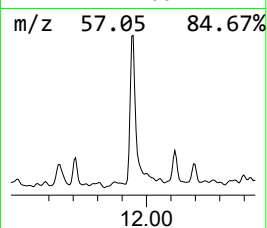
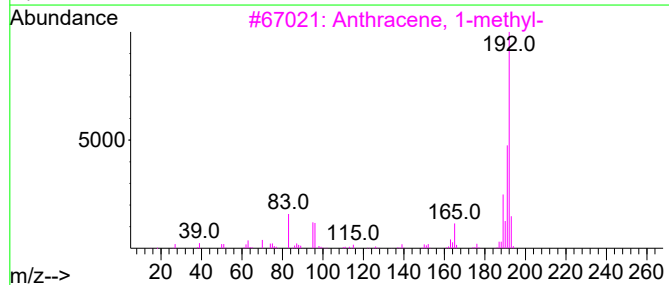
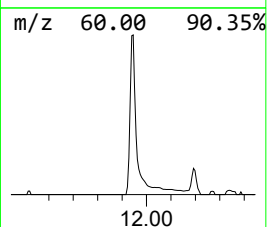
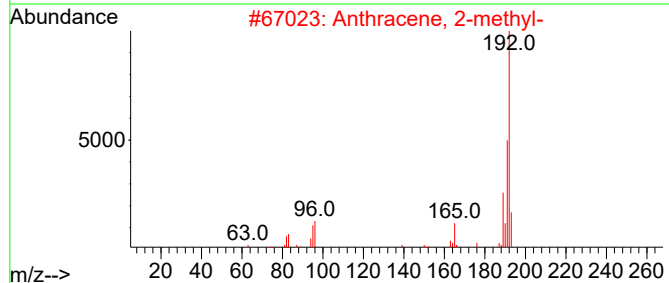
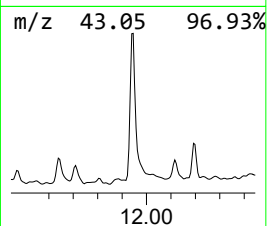
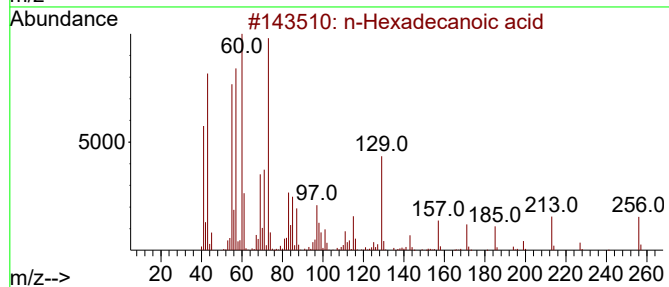
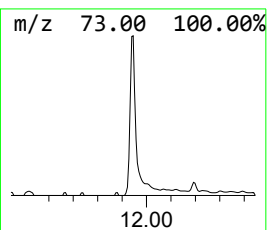
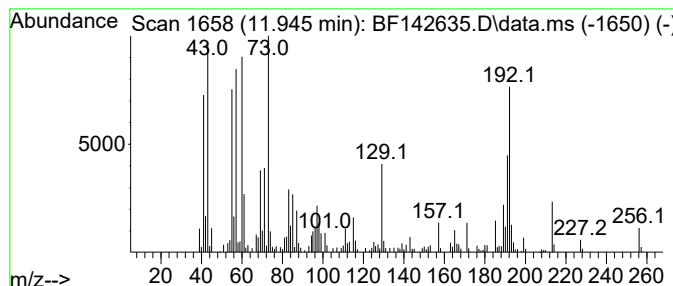
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	6.03 ng	252423	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	70



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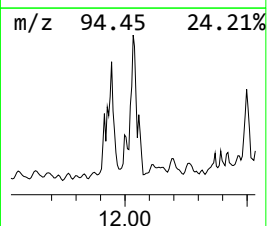
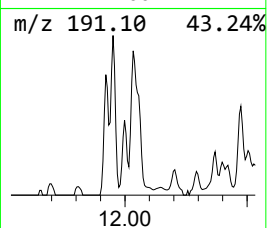
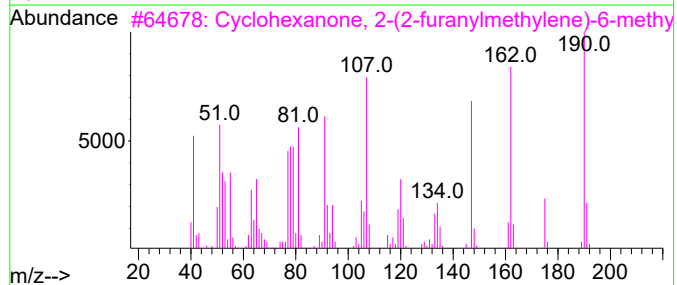
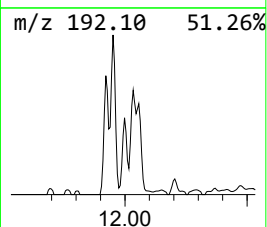
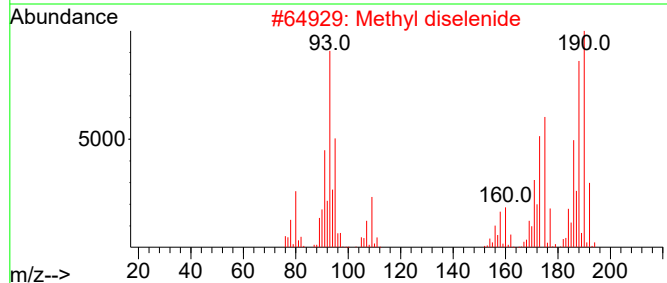
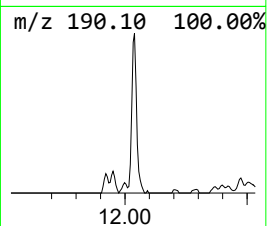
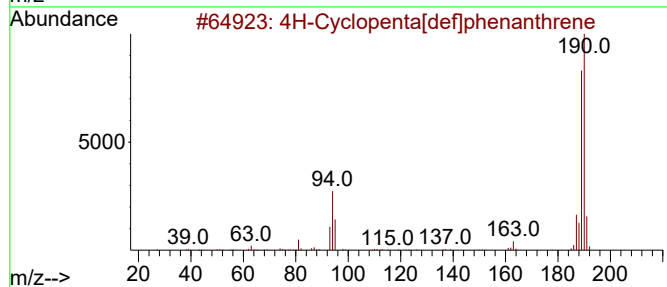
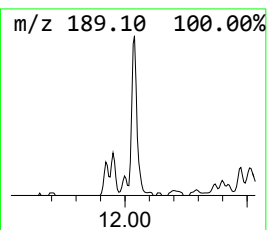
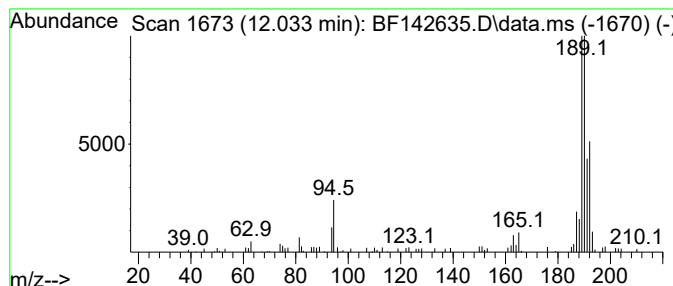
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.033	2.16 ng	90473	Phenanthrene-d10	11.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Methyl diselenide	190	C2H6Se2	007101-31-7	35
3	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	25
5	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	25



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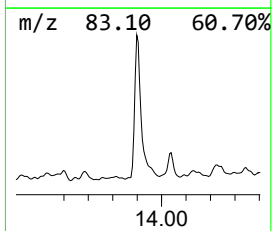
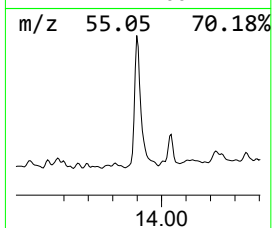
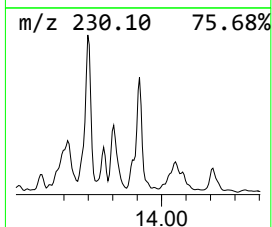
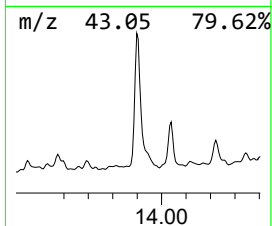
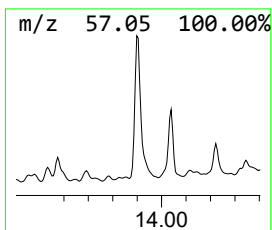
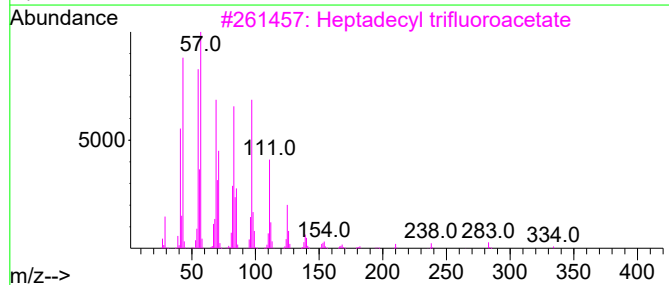
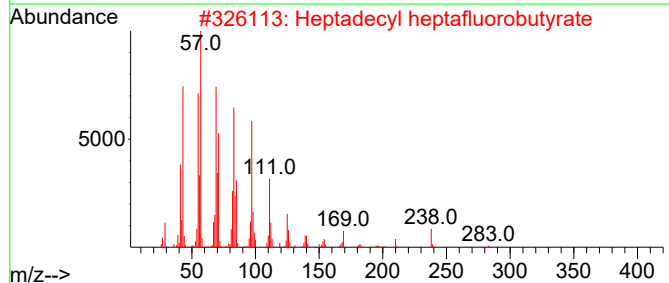
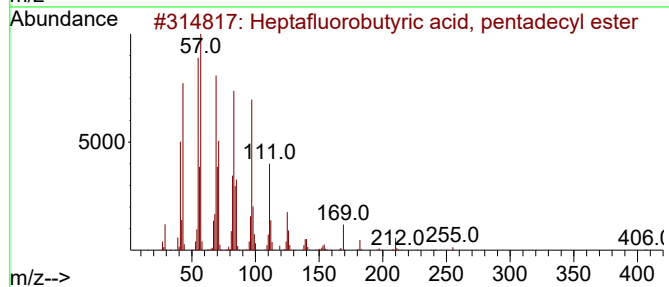
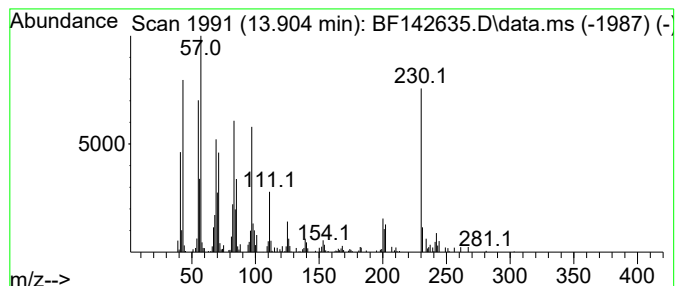
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.26 ng	168011	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	83
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	78
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	64
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060525\
Data File : BF142635.D
Acq On : 05 Jun 2025 15:36
Operator : RC/JU
Sample : Q2199-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11978

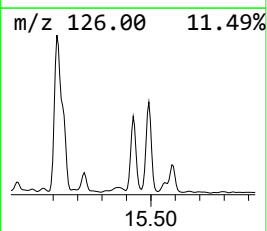
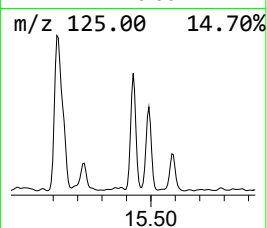
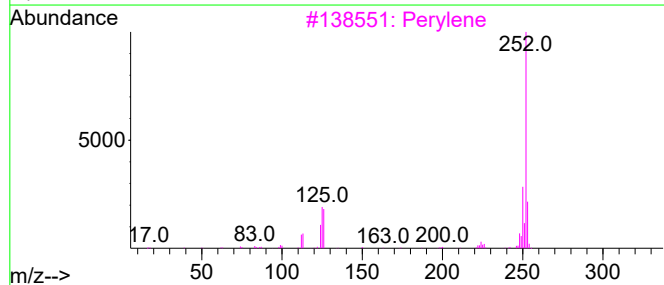
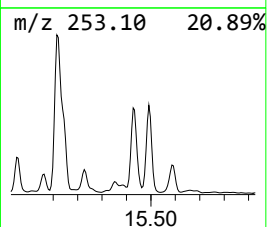
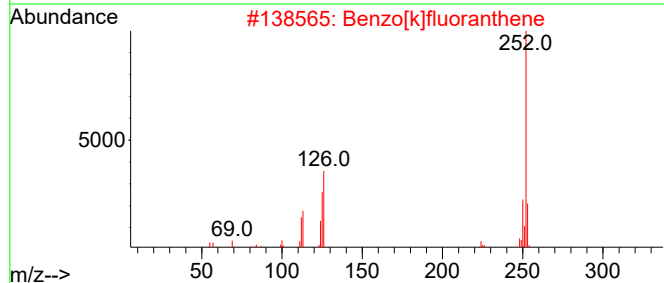
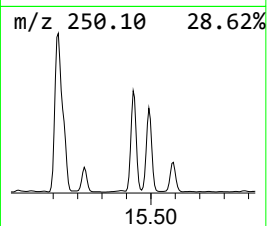
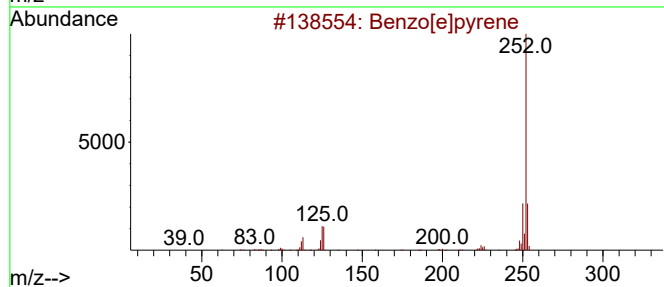
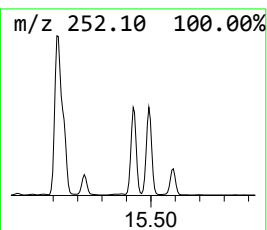
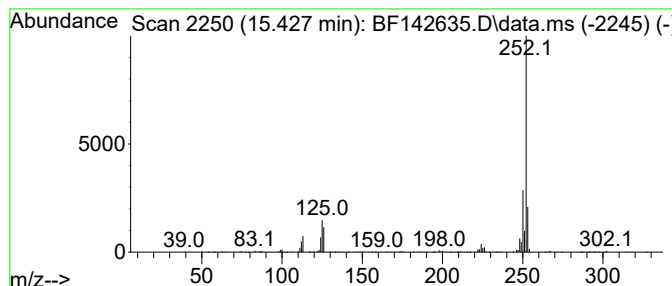
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	7.40 ng	354031	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3			Perylene	252	C20H12	000198-55-0	96
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5			Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060525\
Data File : BF142635.D
Acq On : 05 Jun 2025 15:36
Operator : RC/JU
Sample : Q2199-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

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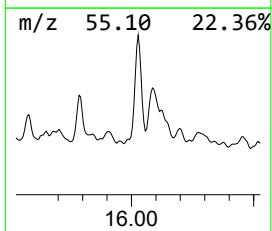
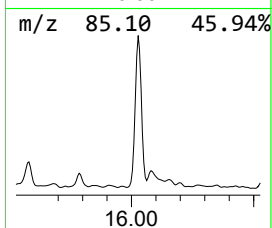
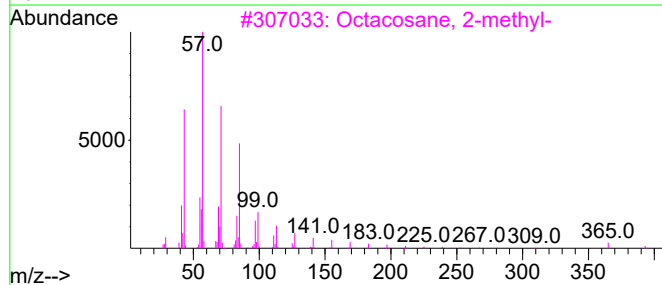
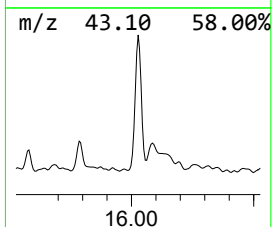
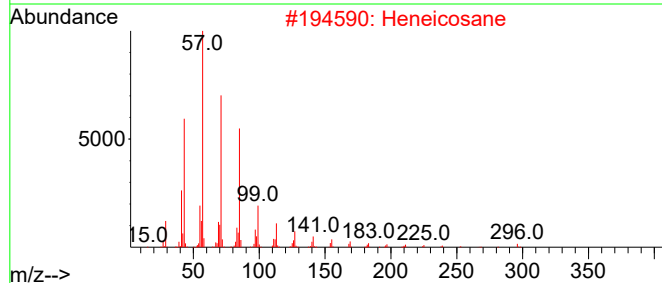
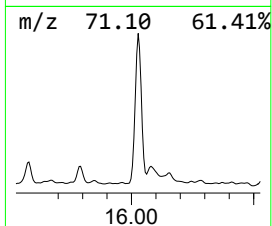
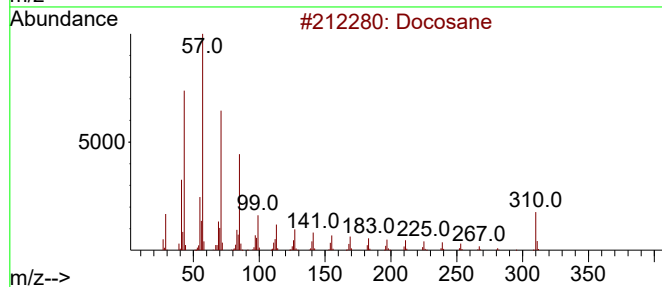
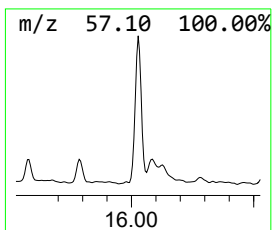
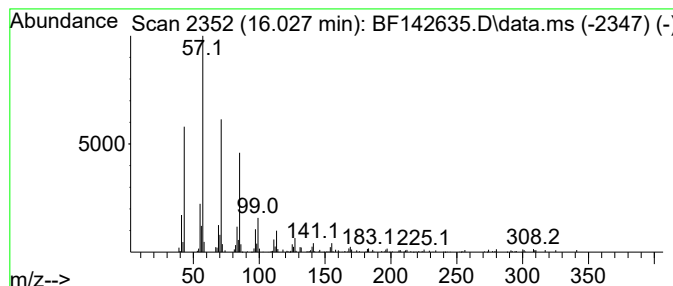
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	3.01 ng	143823	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	93
2			Heneicosane	296	C21H44	000629-94-7	90
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4			Heptadecane, 3-methyl-	254	C18H38	006418-44-6	90
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060525\
Data File : BF142635.D
Acq On : 05 Jun 2025 15:36
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Sample : Q2199-05
Misc :
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Instrument :
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ClientSampleId :
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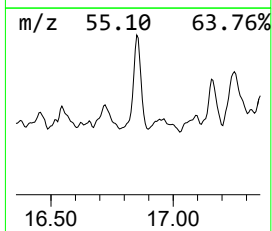
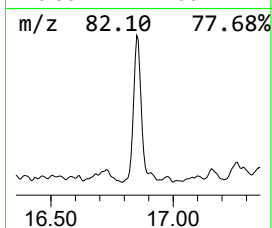
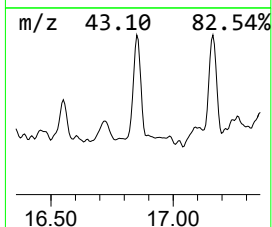
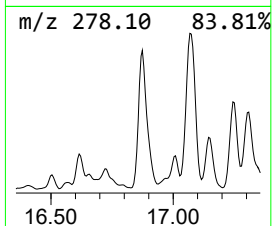
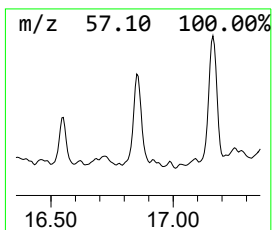
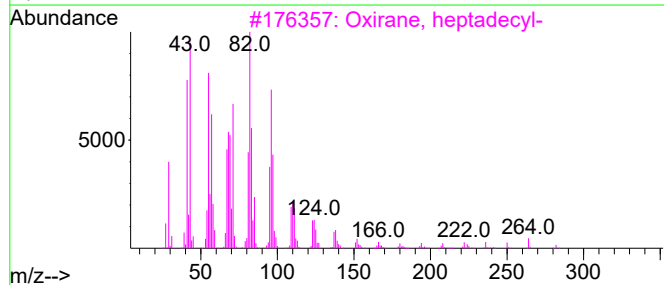
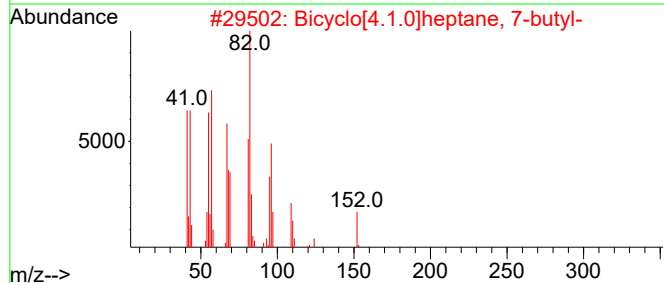
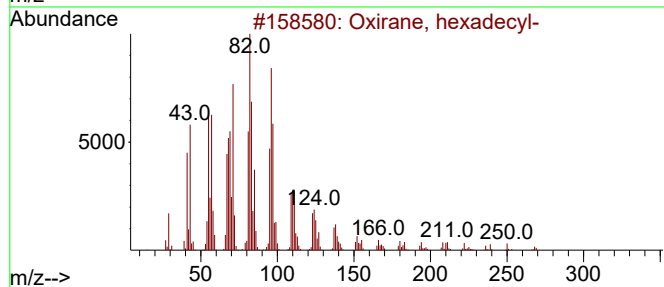
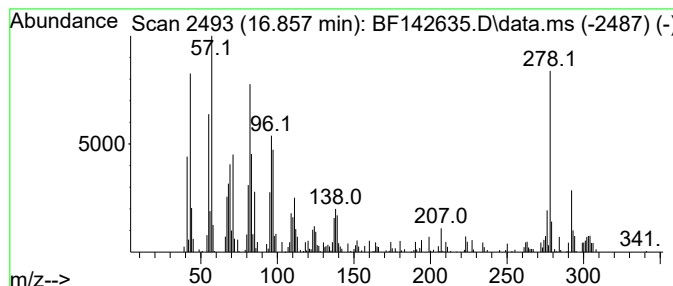
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.857	3.13 ng	149772	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	50
2			Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	42
3			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	41
4			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	41
5			Henicosanal	310	C21H42O	051227-32-8	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060525\
Data File : BF142635.D
Acq On : 05 Jun 2025 15:36
Operator : RC/JU
Sample : Q2199-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

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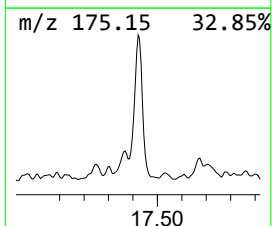
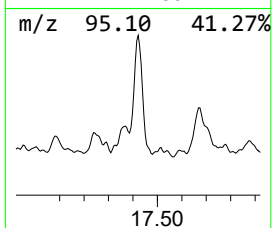
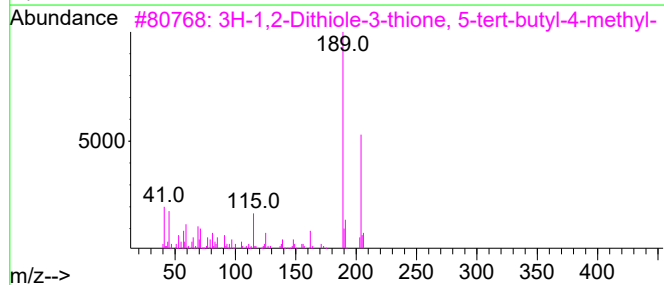
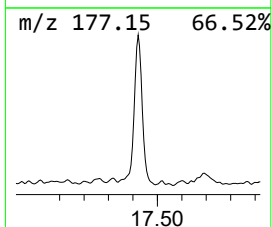
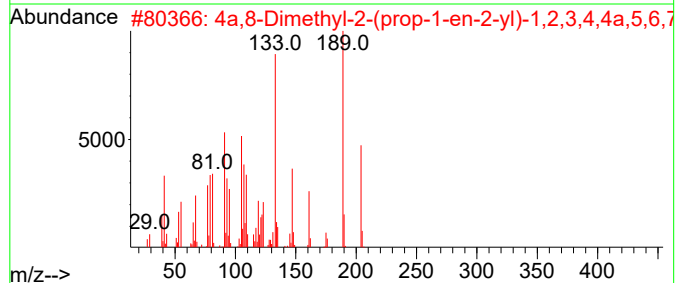
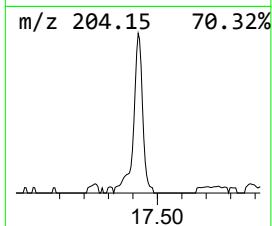
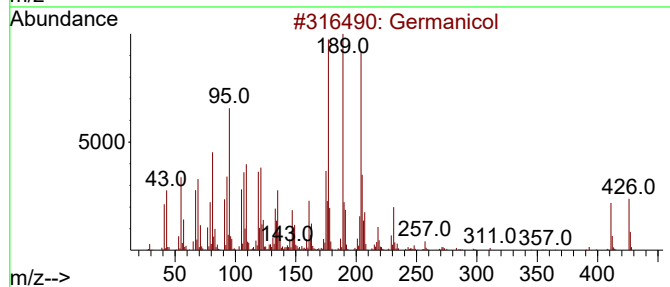
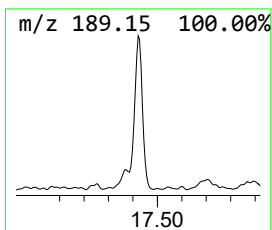
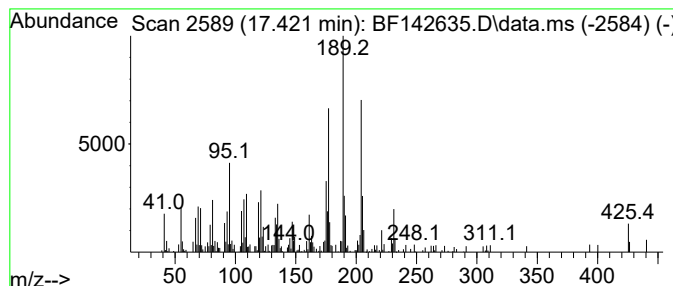
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Germanicol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.421	4.25 ng	203145	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Germanicol	426	C30H50O	000465-02-1	90
2			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	43
3			3H-1,2-Dithiole-3-thione, 5-tert...	204	C8H12S3	013120-76-8	38
4			3,4-Dihydrocoumarin, 4,4,7,8-tet...	204	C13H16O2	040614-36-6	38
5			1H-Indol-6-ylamine, TMS derivative	204	C11H16N2Si	1000484-86-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060525\
Data File : BF142635.D
Acq On : 05 Jun 2025 15:36
Operator : RC/JU
Sample : Q2199-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

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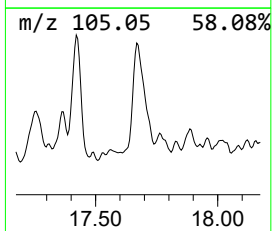
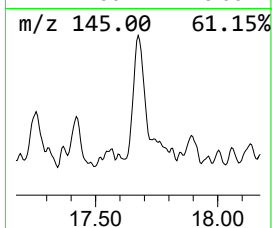
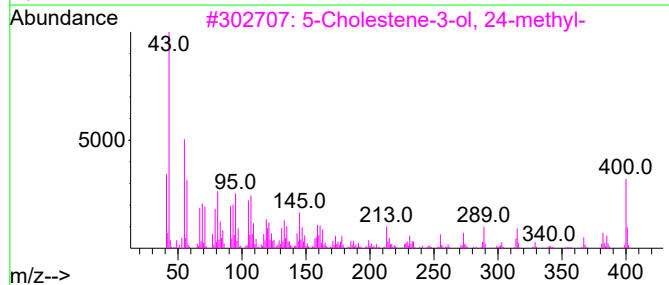
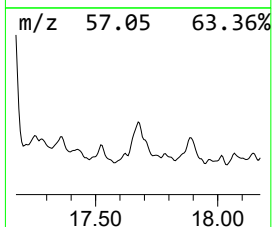
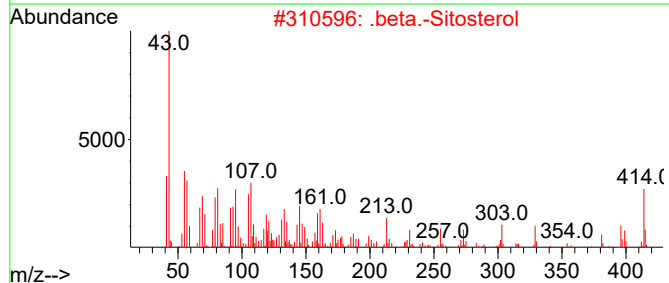
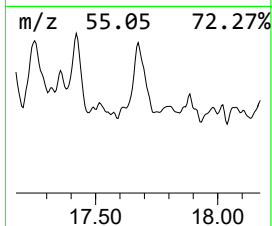
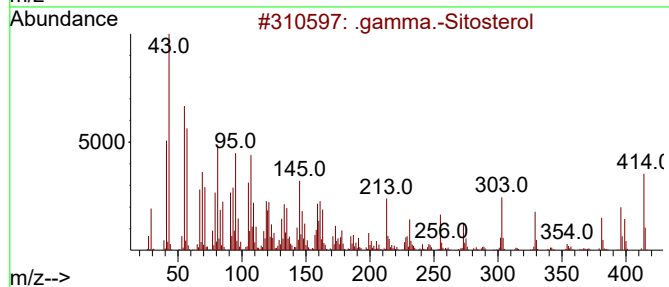
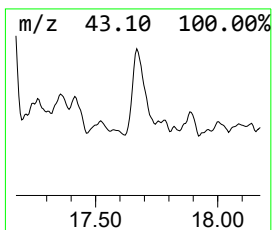
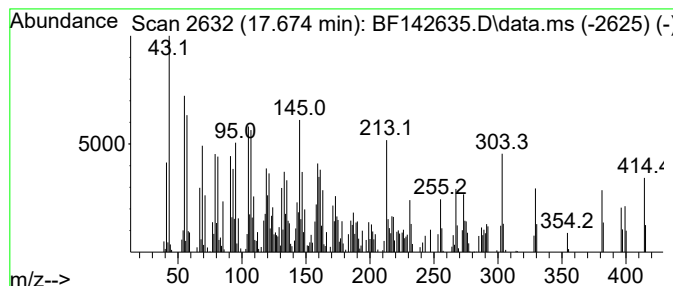
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .gamma.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.674	4.15 ng	198335	Perylene-d12	15.563

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3		5-Cholestene-3-ol, 24-methyl-	400	C28H48O	290299-12-6	38
4		17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	25
5		22,26-Oxido-4,17-cholestadien-3...	414	C27H42O3	1000252-80-4	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060525\
Data File : BF142635.D
Acq On : 05 Jun 2025 15:36
Operator : RC/JU
Sample : Q2199-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052025.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-...	5.110	6.2	ng	225776	1	6.892	724961	20.0
Benzophenone	10.645	9.2	ng	367188	3	9.933	800812	20.0
n-Hexadecanoic ...	11.945	6.0	ng	252423	4	11.422	837162	20.0
4H-Cyclopenta[d]...	12.033	2.2	ng	90473	4	11.422	837162	20.0
Heptafluorobuty...	13.904	2.3	ng	168011	5	14.063	1488670	20.0
Benzo[e]pyrene	15.427	7.4	ng	354031	6	15.563	956939	20.0
Docosane	16.027	3.0	ng	143823	6	15.563	956939	20.0
Oxirane, hexade...	16.857	3.1	ng	149772	6	15.563	956939	20.0
Germanicol	17.421	4.3	ng	203145	6	15.563	956939	20.0
.gamma.-Sitosterol	17.674	4.2	ng	198335	6	15.563	956939	20.0