

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
 Data File : BF141206.D
 Acq On : 17 Jan 2025 21:11
 Operator : RC/JU
 Sample : Q1115-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-214

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-BF011025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141206.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	6	16	27	rVB	95401	154938	2.96%	0.401%
2	5.028	487	499	508	rVB	258310	446698	8.53%	1.157%
3	5.428	560	567	572	rBV	3270429	4555370	86.97%	11.799%
4	6.440	732	739	745	rBV	3153068	4647969	88.73%	12.039%
5	6.810	797	802	807	rBV	945322	1149603	21.95%	2.978%
6	7.375	890	898	903	rBV	2132653	3053153	58.29%	7.908%
7	7.628	936	941	948	rVB	132590	164297	3.14%	0.426%
8	8.092	1014	1020	1030	rBV	1190140	1560017	29.78%	4.041%
9	8.310	1051	1057	1063	rVB	54389	73533	1.40%	0.190%
10	9.163	1196	1202	1208	rBV	3879773	5238044	100.00%	13.567%
11	9.845	1311	1318	1322	rBV	1220565	1620578	30.94%	4.198%
12	10.045	1348	1352	1356	rBV	45954	58575	1.12%	0.152%
13	10.251	1382	1387	1394	rBV2	35643	58586	1.12%	0.152%
14	10.386	1406	1410	1416	rVB	55783	73058	1.39%	0.189%
15	10.557	1434	1439	1444	rVB	324595	410286	7.83%	1.063%
16	10.633	1445	1452	1457	rBV	2295539	3082135	58.84%	7.983%
17	10.810	1478	1482	1485	rBV	38551	53160	1.01%	0.138%
18	11.192	1541	1547	1550	rBV5	27523	55460	1.06%	0.144%
19	11.327	1565	1570	1578	rBV2	1045153	1859145	35.49%	4.815%
20	11.398	1578	1582	1586	rVB	79223	105583	2.02%	0.273%
21	11.557	1603	1609	1617	rBV2	45772	81983	1.57%	0.212%
22	11.827	1651	1655	1656	rBV	55474	59493	1.14%	0.154%
23	11.857	1656	1660	1666	rVB	557411	758265	14.48%	1.964%
24	11.939	1671	1674	1683	rVB2	89647	177343	3.39%	0.459%
25	12.127	1701	1706	1715	rVB2	43221	96414	1.84%	0.250%
26	12.539	1771	1776	1782	rBV	469110	614625	11.73%	1.592%
27	12.645	1789	1794	1800	rBV2	109167	181120	3.46%	0.469%
28	12.769	1808	1815	1819	rBV	384176	585173	11.17%	1.516%
29	12.916	1832	1840	1845	rBV	2896737	3717738	70.98%	9.629%
30	12.986	1848	1852	1860	rVV3	31668	62890	1.20%	0.163%
31	13.098	1868	1871	1874	rVB	54225	65610	1.25%	0.170%
32	13.198	1885	1888	1891	rBV	43274	60142	1.15%	0.156%
33	13.715	1972	1976	1979	rBV2	39822	67052	1.28%	0.174%
34	13.815	1989	1993	2001	rVB2	222409	338326	6.46%	0.876%
35	13.968	2013	2019	2029	rBV2	941426	1627250	31.07%	4.215%
36	14.998	2190	2194	2203	rVB	180223	395080	7.54%	1.023%

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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 >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.298	2241	2245	2250	rVB	90174	131220	2.51%	0.340%
38	15.357	2251	2255	2260	rVV	112848	166659	3.18%	0.432%
39	15.421	2261	2266	2277	rVB	597796	1001503	19.12%	2.594%

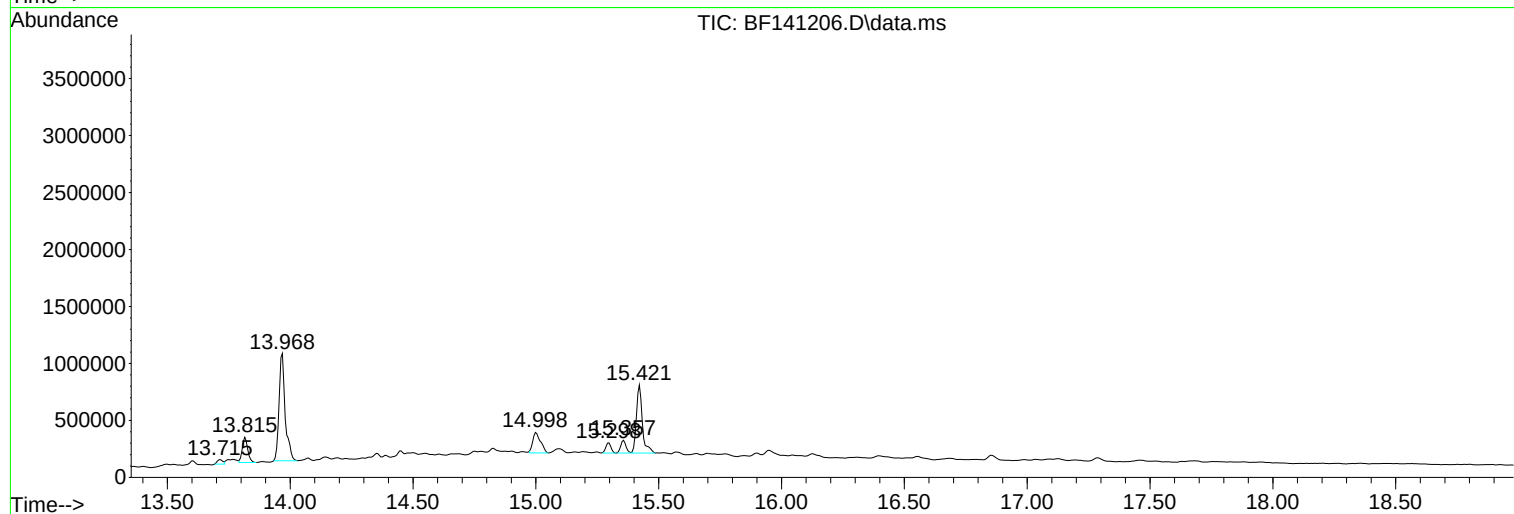
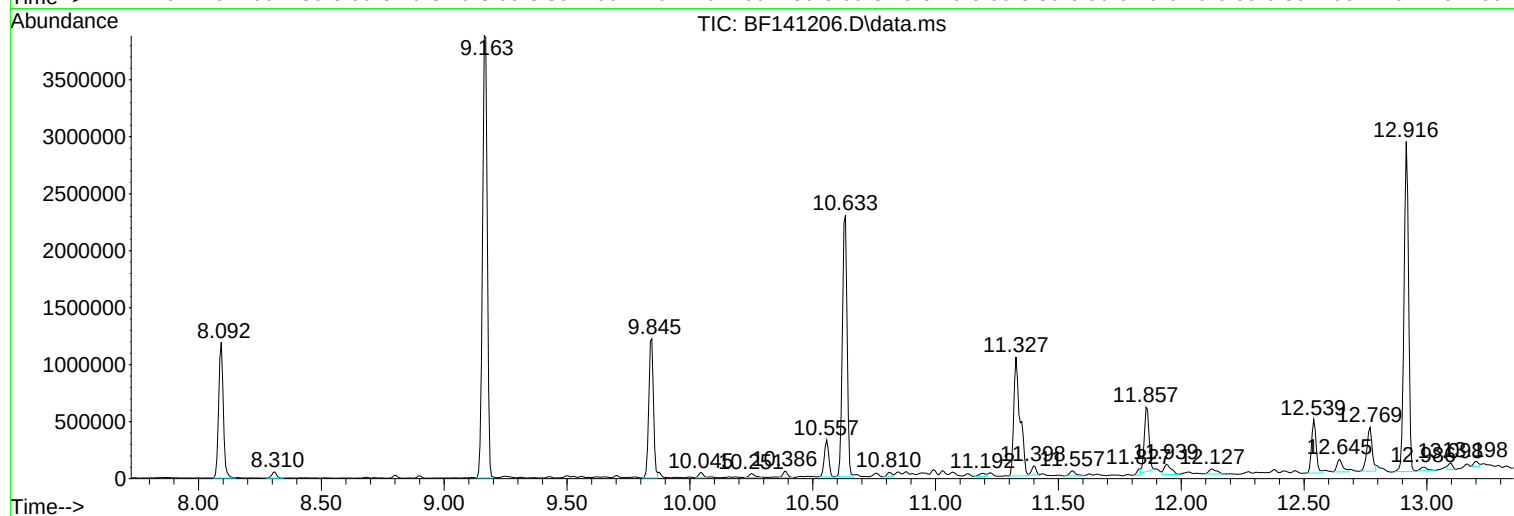
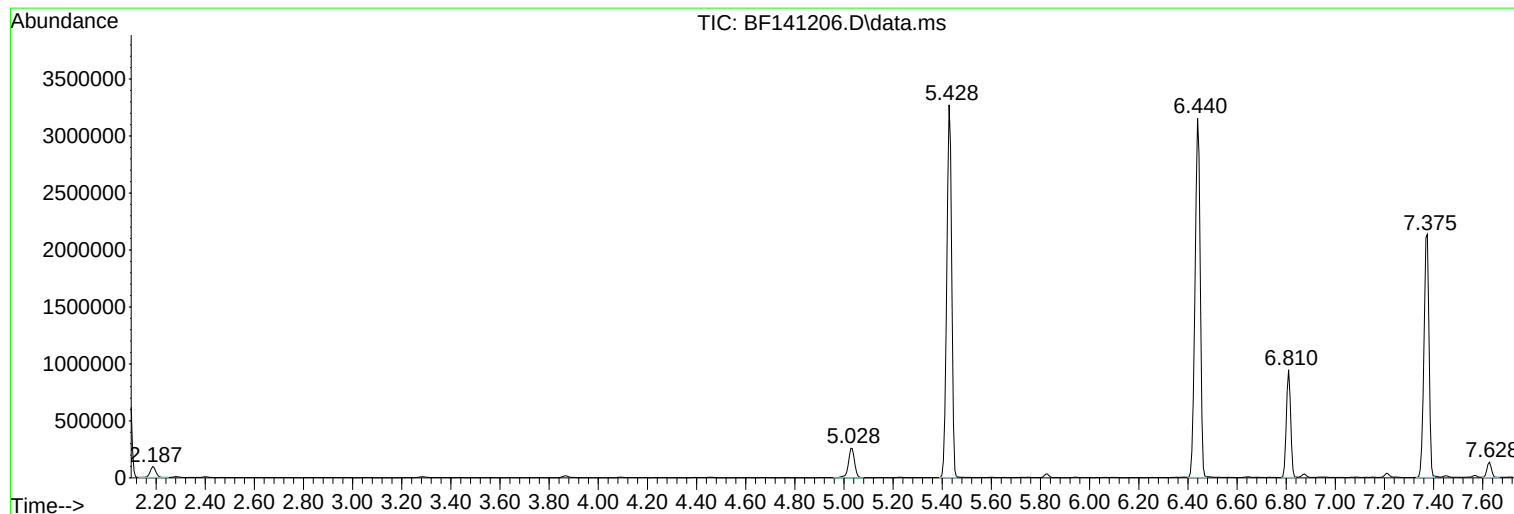
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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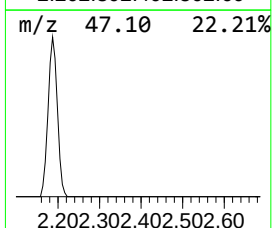
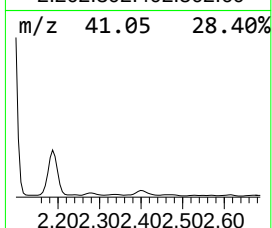
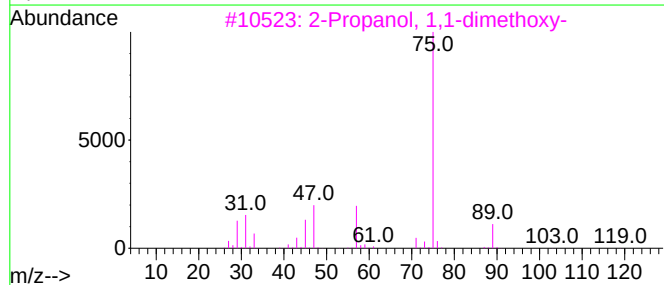
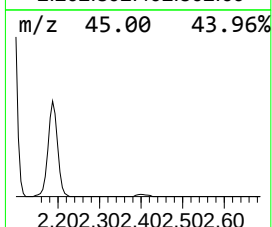
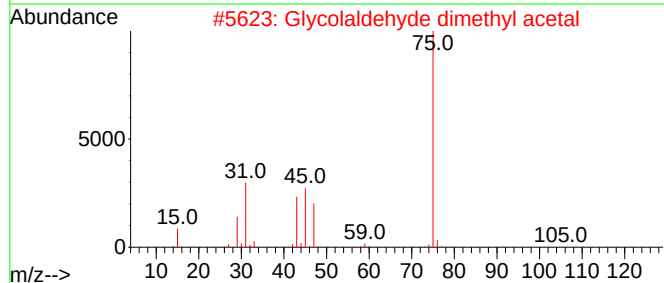
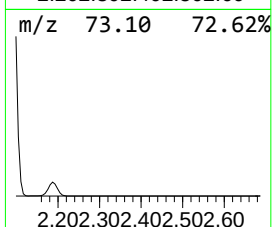
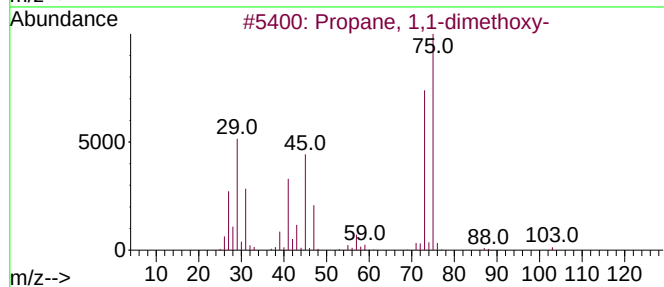
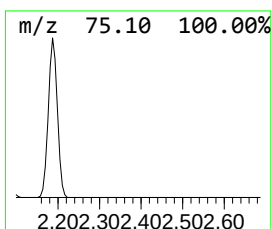
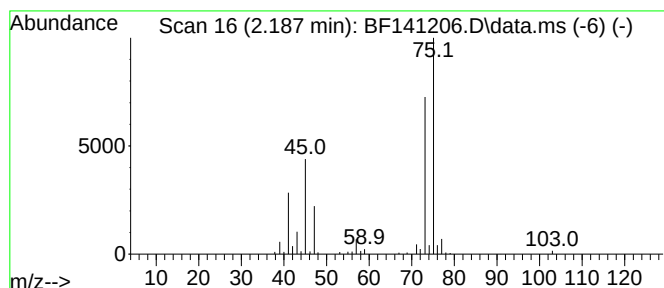
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	2.70 ng	154938	1,4-Dichlorobenzene-d4	6.810

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	45
3		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	40
4		Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	36
5		Ethanethioamide	75	C2H5NS	000062-55-5	25



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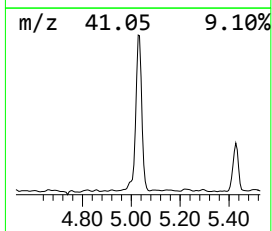
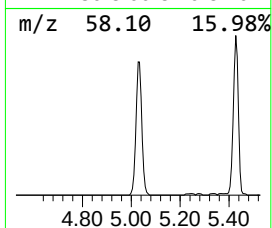
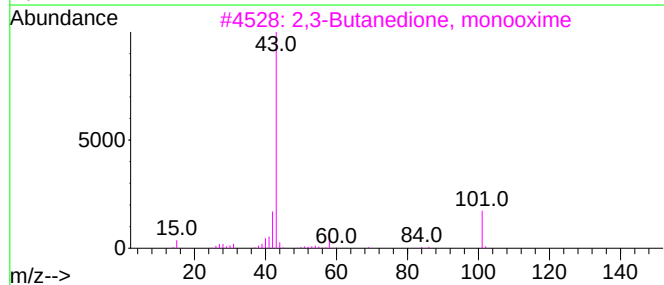
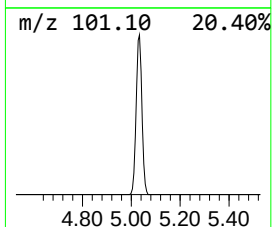
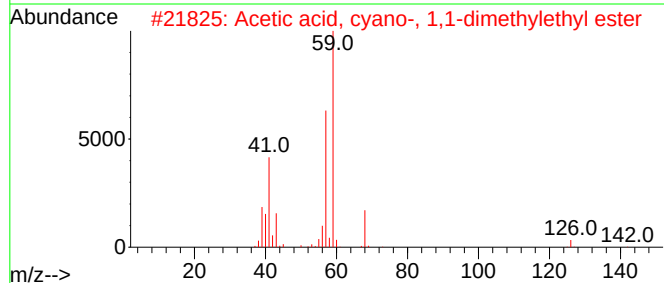
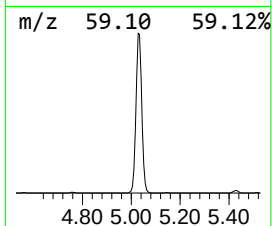
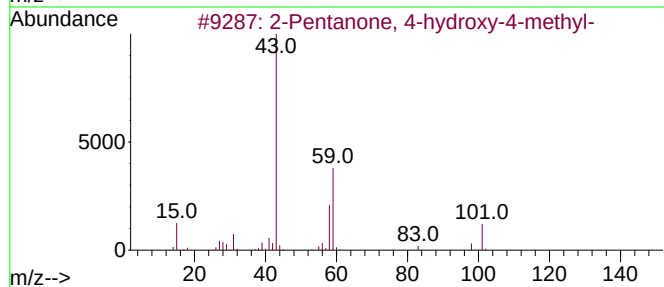
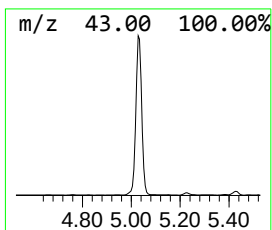
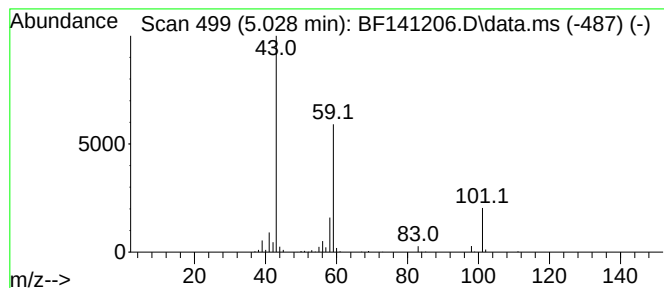
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	7.77 ng	446698	1,4-Dichlorobenzene-d4	6.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
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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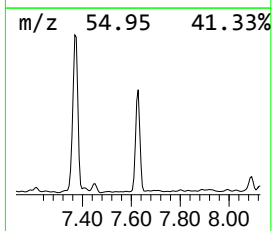
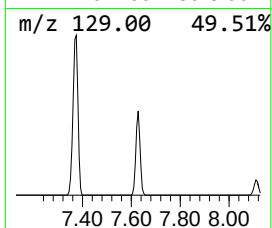
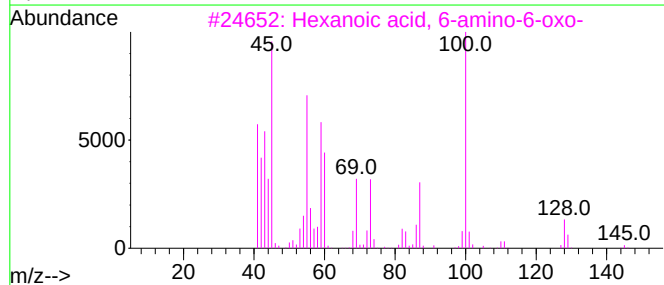
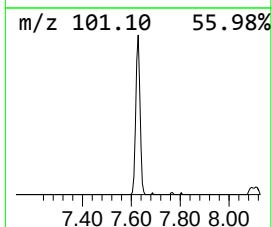
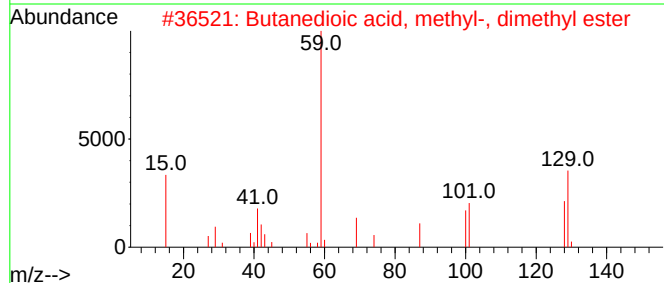
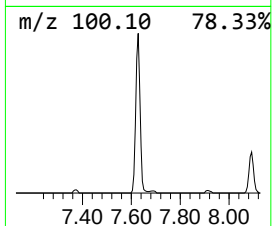
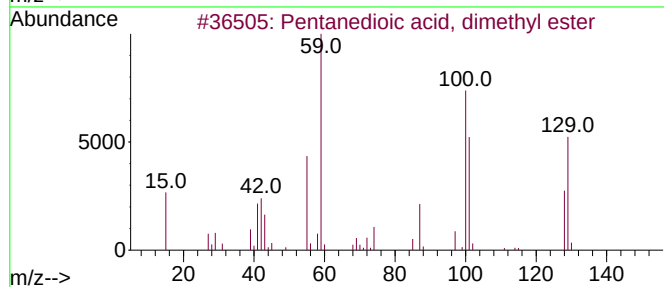
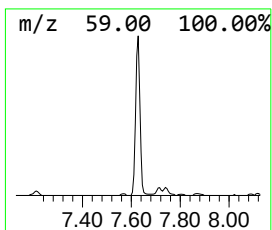
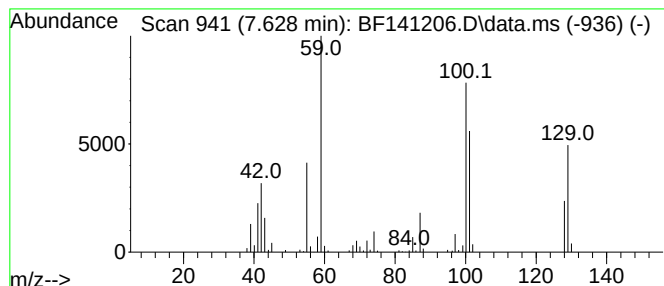
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.628	2.11 ng	164297	Naphthalene-d8	8.092

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	47
3			Hexanoic acid, 6-amino-6-oxo-	145	C6H11NO3	000334-25-8	25
4			Propanal, 2-methyl-, methylhydra...	100	C5H12N2	016713-37-4	25
5			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	17



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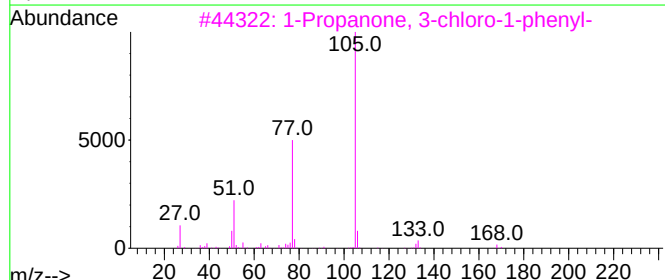
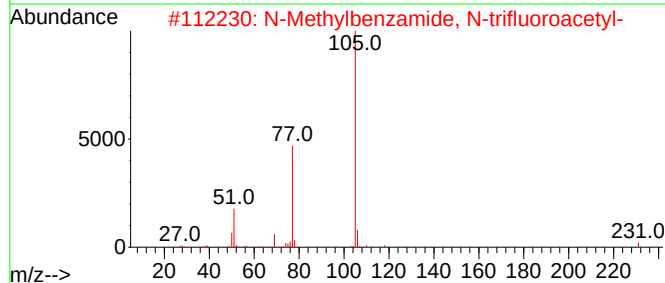
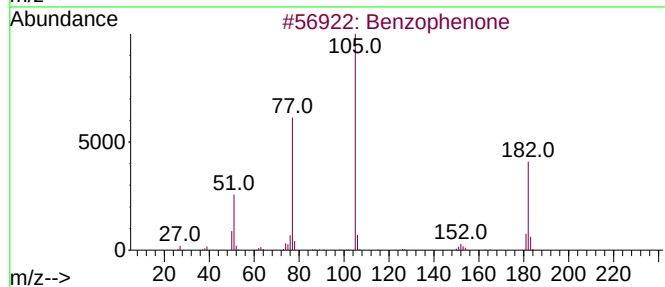
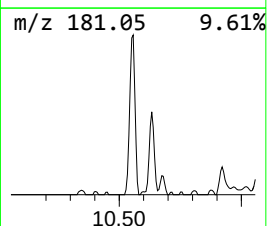
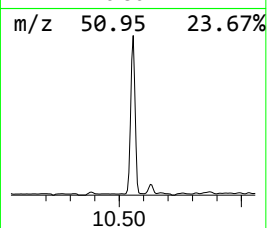
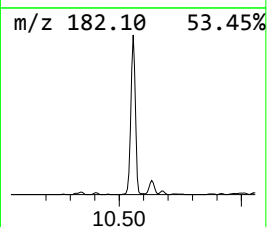
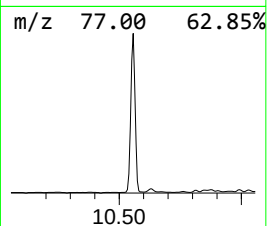
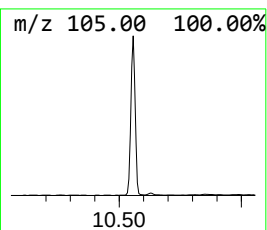
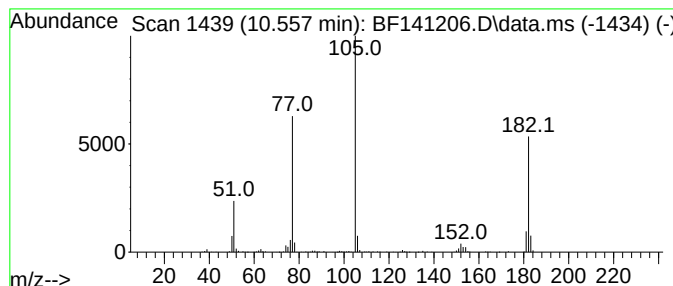
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Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.557	5.06 ng	410286	Acenaphthene-d10	9.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			Benzoyl bromide	184	C7H5BrO	000618-32-6	47



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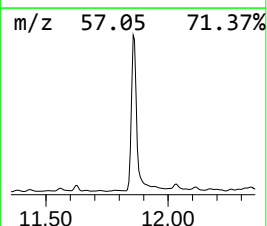
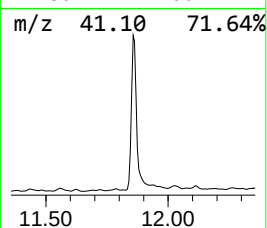
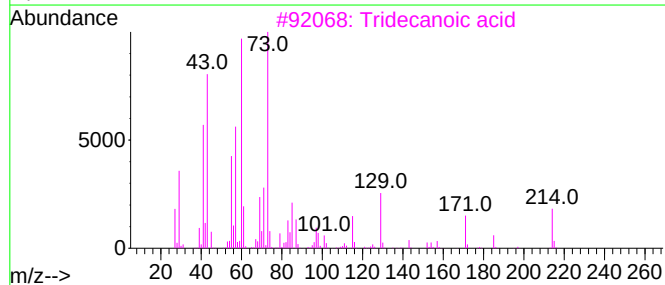
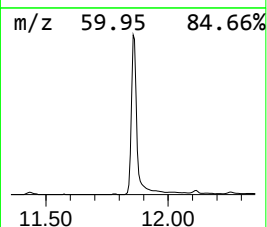
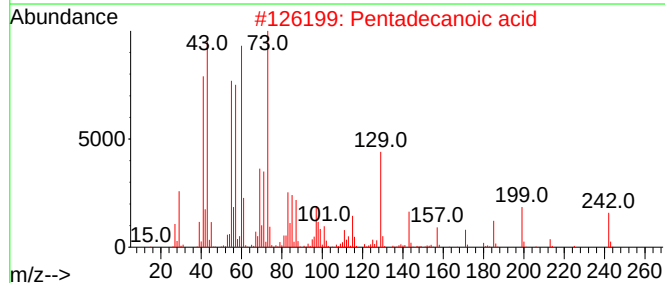
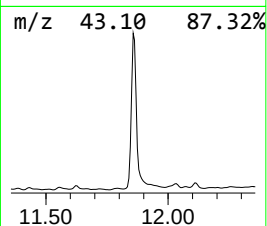
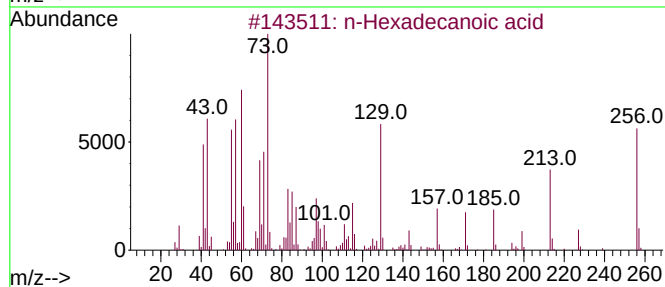
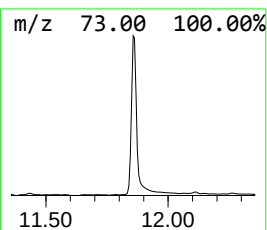
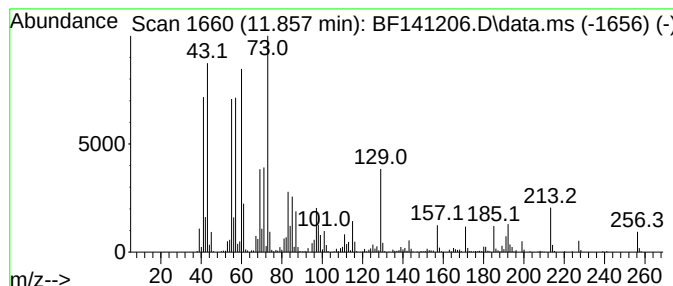
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	8.16 ng	758265	Phenanthrene-d10	11.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141206.D
Acq On : 17 Jan 2025 21:11
Operator : RC/JU
Sample : Q1115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-214

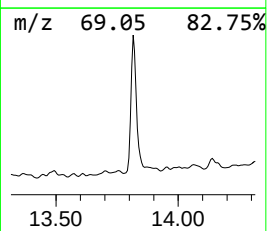
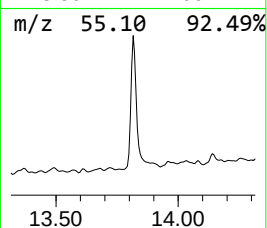
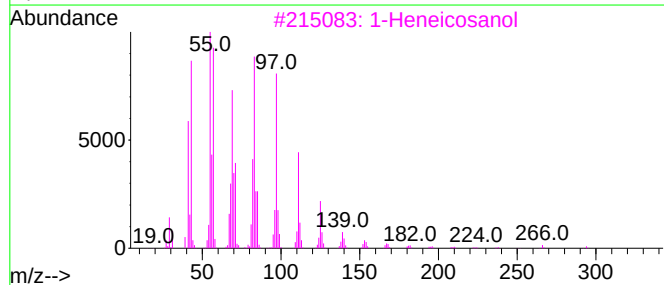
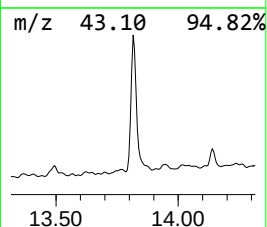
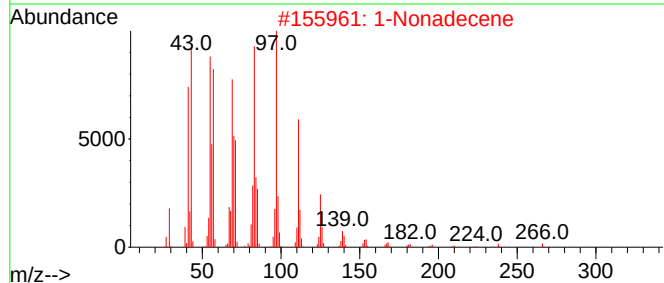
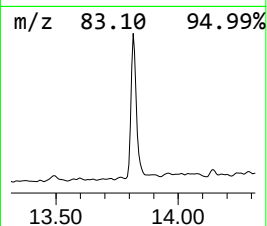
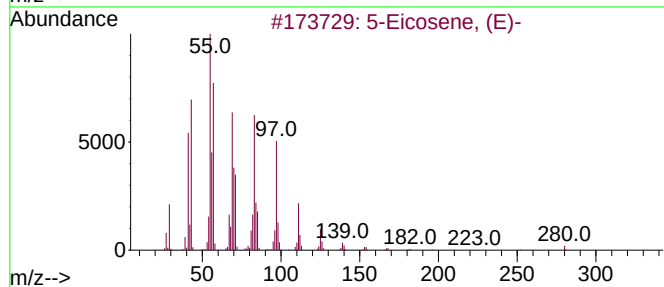
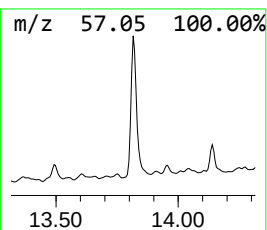
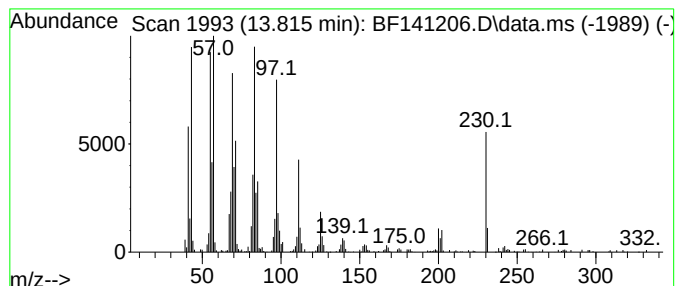
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	4.16 ng	338326	Chrysene-d12	13.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		1-Nonadecene	266	C19H38	018435-45-5	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141206.D
Acq On : 17 Jan 2025 21:11
Operator : RC/JU
Sample : Q1115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-214

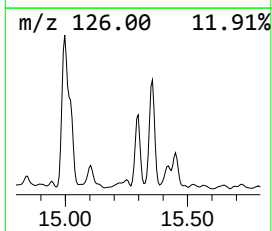
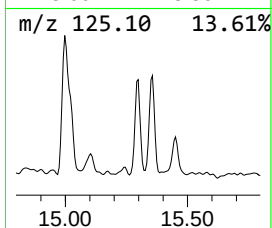
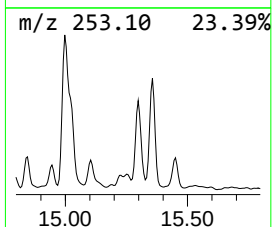
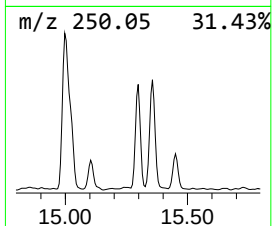
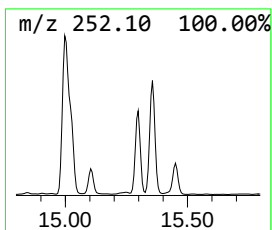
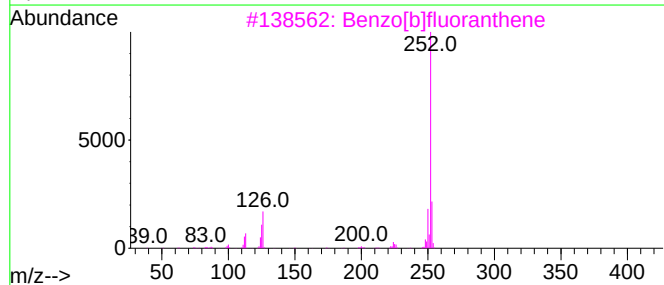
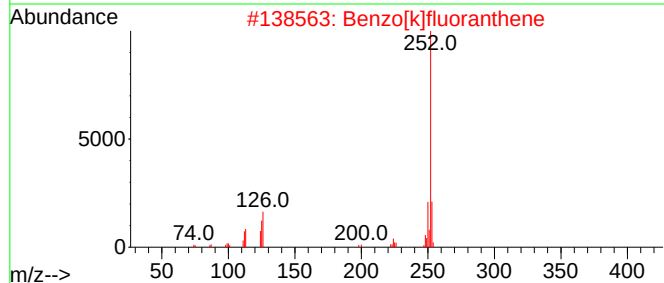
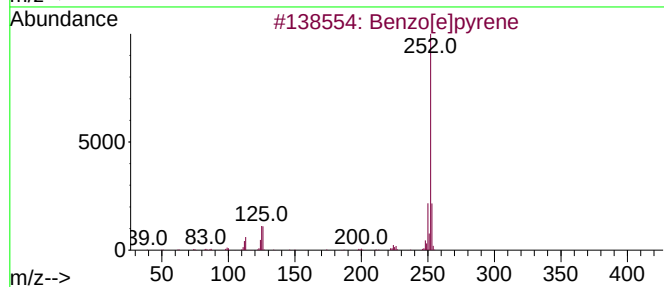
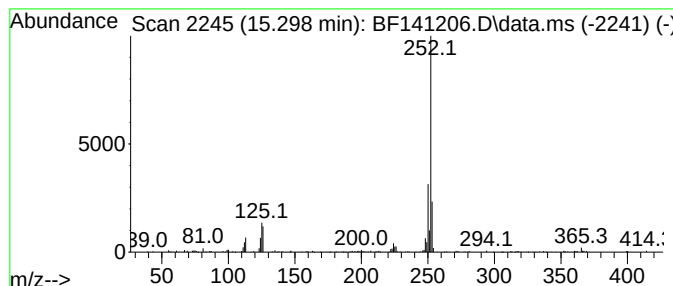
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	2.62 ng	131220	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	97
4			Perylene	252	C20H12	000198-55-0	96
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011725\
Data File : BF141206.D
Acq On : 17 Jan 2025 21:11
Operator : RC/JU
Sample : Q1115-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-214

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-di...	2.187	2.7	ng	154938	1	6.810	1149600	20.0
2-Pentanone, 4-...	5.028	7.8	ng	446698	1	6.810	1149600	20.0
Pentanedioic ac...	7.628	2.1	ng	164297	2	8.092	1560020	20.0
Benzophenone	10.557	5.1	ng	410286	3	9.845	1620580	20.0
n-Hexadecanoic ...	11.857	8.2	ng	758265	4	11.327	1859150	20.0
5-Eicosene, (E)-	13.816	4.2	ng	338326	5	13.968	1627250	20.0
Benzo[e]pyrene	15.298	2.6	ng	131220	6	15.421	1001500	20.0