

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
 Data File : BF139987.D
 Acq On : 24 Oct 2024 02:06
 Operator : RC/JU
 Sample : P4486-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EO-03-102224

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139987.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	7	15	22	rVB	656655	1031141	40.74%	4.639%
2	5.116	509	514	521	rVB	27968	42504	1.68%	0.191%
3	5.504	574	580	586	rBV	1912986	2531224	100.00%	11.389%
4	5.628	597	601	608	rVB	29160	45072	1.78%	0.203%
5	5.992	659	663	667	rBV	98856	135045	5.34%	0.608%
6	6.128	678	686	697	rBV3	23831	56593	2.24%	0.255%
7	6.269	706	710	712	rBV	46062	63507	2.51%	0.286%
8	6.292	712	714	718	rVB	59712	63032	2.49%	0.284%
9	6.457	733	742	745	rBV	20216	34722	1.37%	0.156%
10	6.510	745	751	764	rVB	1744374	2394058	94.58%	10.772%
11	6.892	810	816	821	rBV	624465	780930	30.85%	3.514%
12	7.445	902	910	915	rBV	1146998	1505269	59.47%	6.773%
13	7.698	949	953	958	rVB	78332	95221	3.76%	0.428%
14	8.169	1027	1033	1046	rBV	722900	932155	36.83%	4.194%
15	8.380	1065	1069	1074	rBV	27703	37222	1.47%	0.167%
16	9.245	1210	1216	1221	rBV	1955222	2418261	95.54%	10.880%
17	9.322	1226	1229	1237	rVB2	14920	25664	1.01%	0.115%
18	9.927	1326	1332	1341	rBV	674413	889968	35.16%	4.004%
19	10.639	1448	1453	1460	rBV	449493	571880	22.59%	2.573%
20	10.710	1460	1465	1478	rVV	1063689	1370598	54.15%	6.167%
21	10.833	1482	1486	1491	rVB3	21464	38274	1.51%	0.172%
22	10.945	1501	1505	1510	rVB	72110	88842	3.51%	0.400%
23	11.069	1522	1526	1531	rBV3	25909	36536	1.44%	0.164%
24	11.410	1579	1584	1593	rBV2	688139	1017254	40.19%	4.577%
25	11.480	1593	1596	1599	rVV2	24243	30444	1.20%	0.137%
26	11.857	1657	1660	1664	rBV3	32069	53046	2.10%	0.239%
27	11.939	1669	1674	1684	rVV	497802	760369	30.04%	3.421%
28	12.498	1766	1769	1775	rVB3	52094	89732	3.55%	0.404%
29	12.627	1787	1791	1803	rBV	156298	299161	11.82%	1.346%
30	12.721	1803	1807	1814	rBV	125434	217952	8.61%	0.981%
31	12.851	1826	1829	1836	rBV	128128	196725	7.77%	0.885%
32	12.998	1849	1854	1861	rVB	1967612	2505374	98.98%	11.272%
33	13.898	2004	2007	2017	rVB2	204027	368315	14.55%	1.657%
34	14.051	2029	2033	2040	rBV	609865	842688	33.29%	3.792%
35	15.533	2282	2285	2297	rVB	351443	656911	25.95%	2.956%

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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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

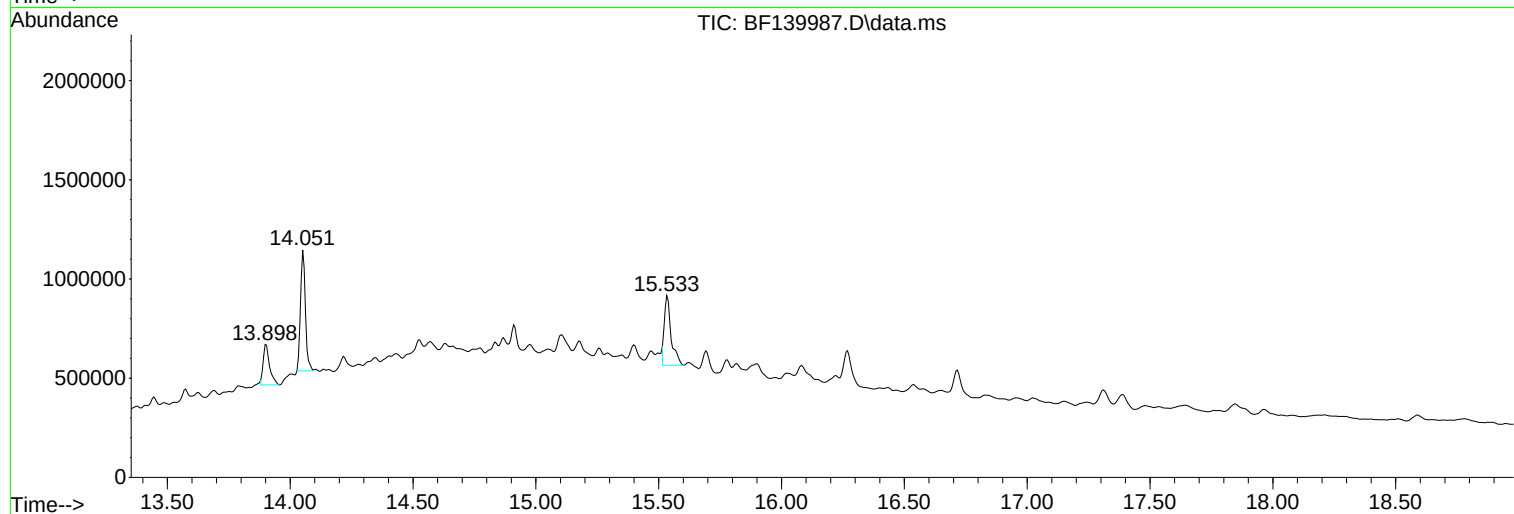
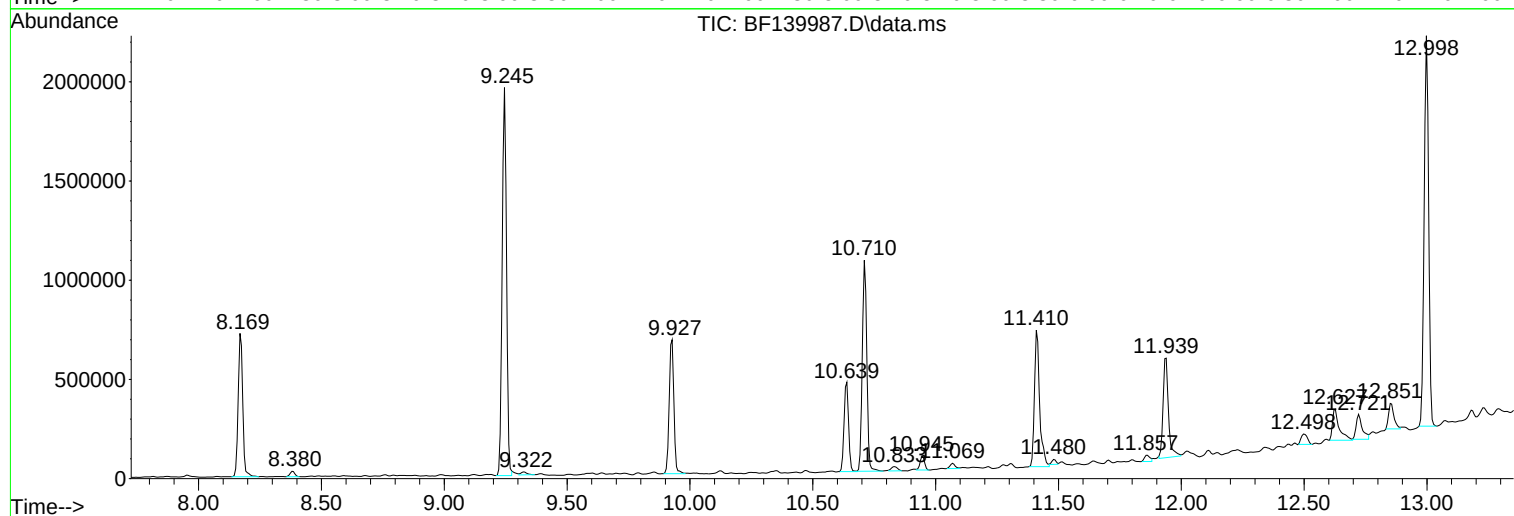
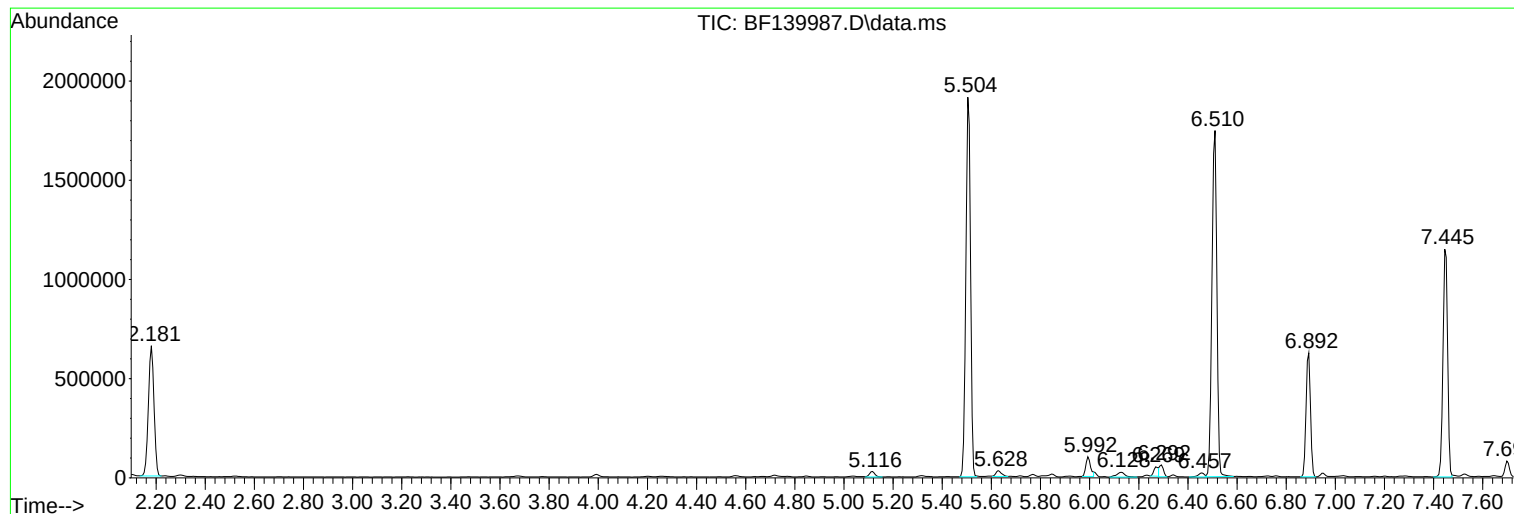
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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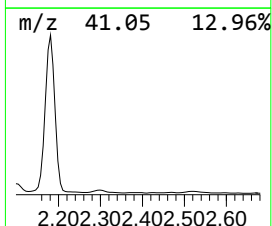
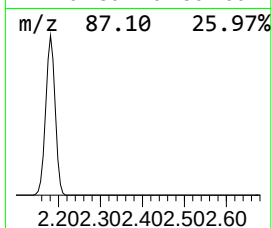
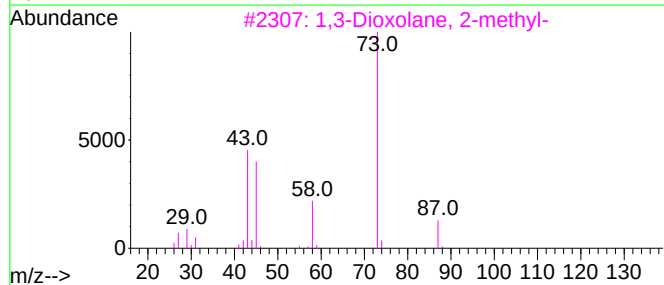
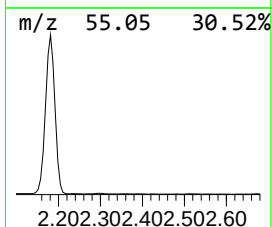
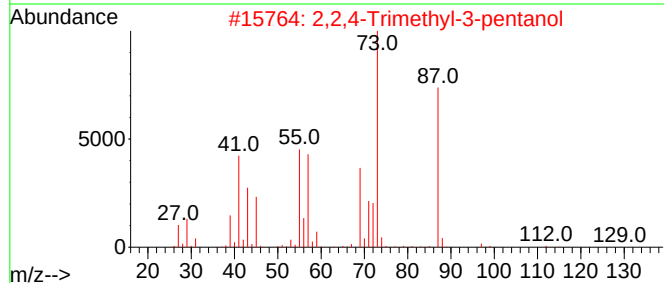
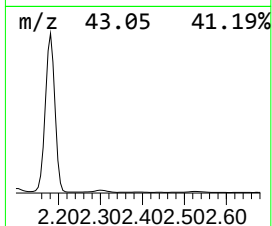
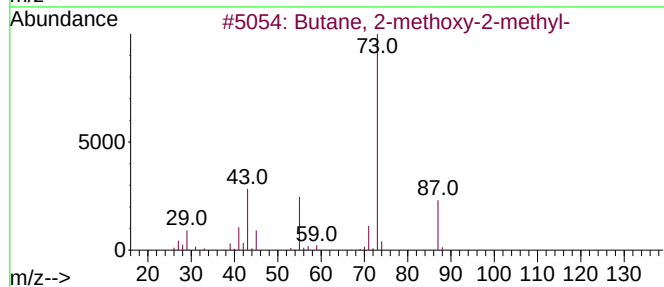
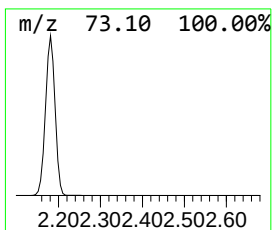
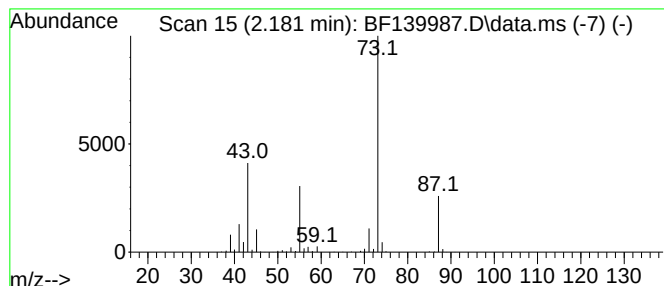
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	26.41 ng	1031140	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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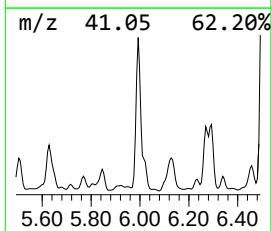
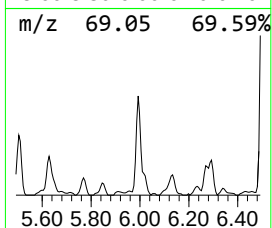
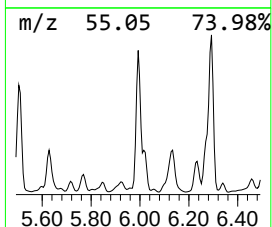
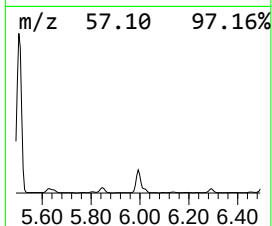
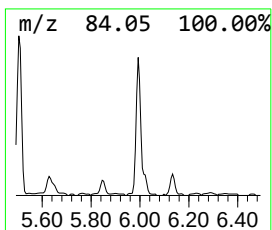
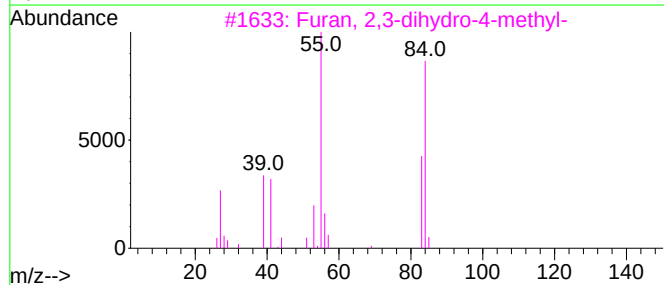
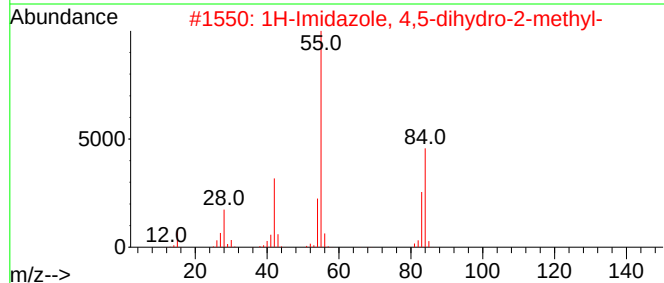
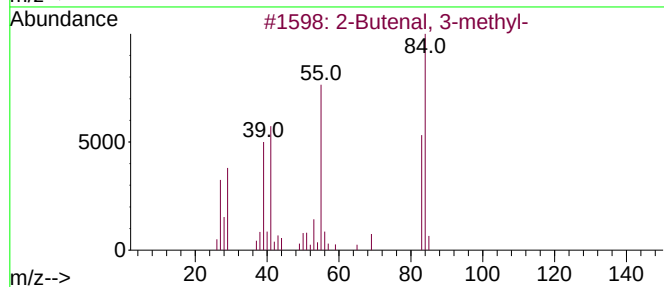
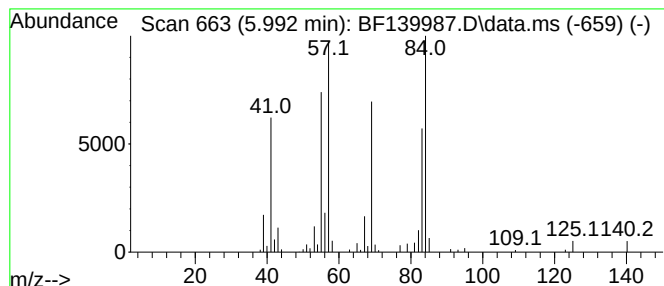
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Butenal, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.992	3.46 ng	135045	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	53
2			1H-Imidazole, 4,5-dihydro-2-methyl-	84	C4H8N2	000534-26-9	50
3			Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	47
4			Cyclopentanone, 2-ethyl-	112	C7H12O	004971-18-0	45
5			3-Hexene	84	C6H12	000592-47-2	43



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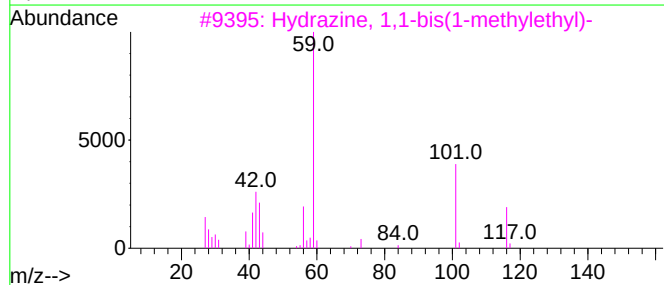
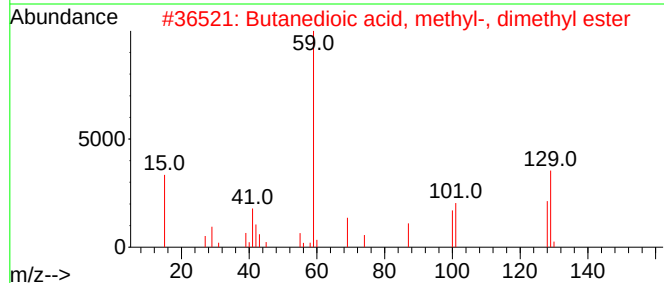
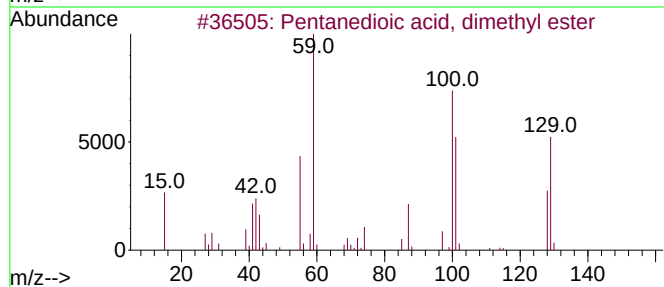
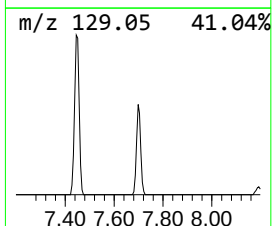
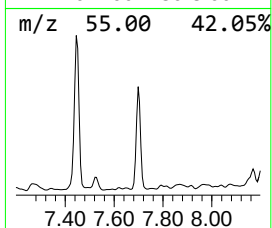
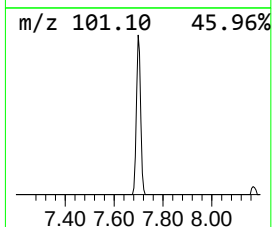
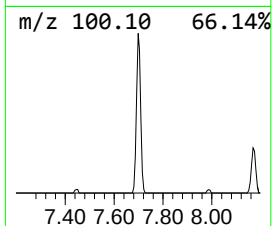
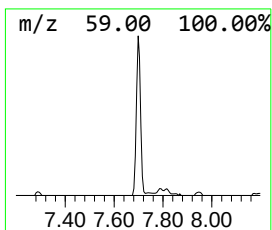
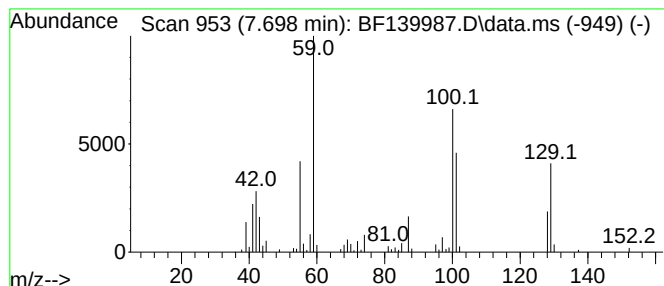
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	2.04 ng	95221	Naphthalene-d8	8.169

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	53
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	37
4			Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	32
5			Oxirane, tetramethyl-	100	C6H12O	005076-20-0	27



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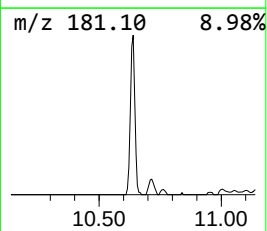
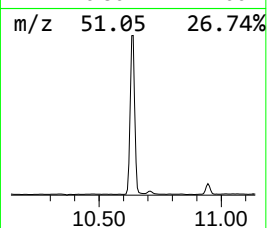
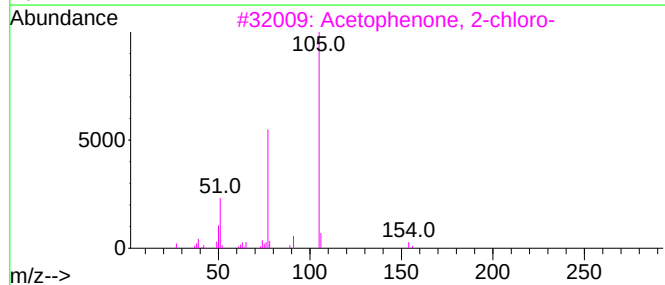
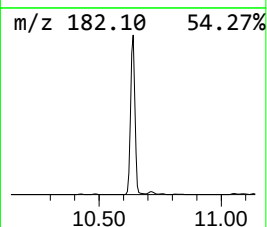
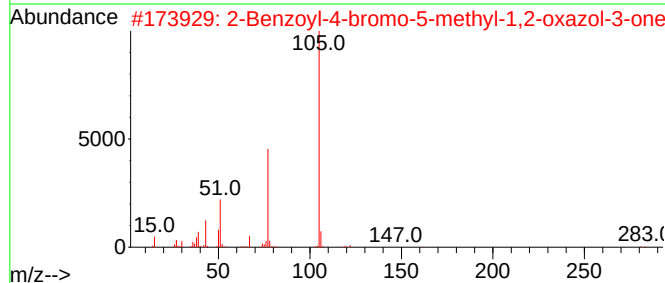
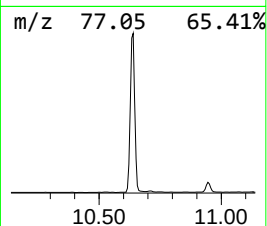
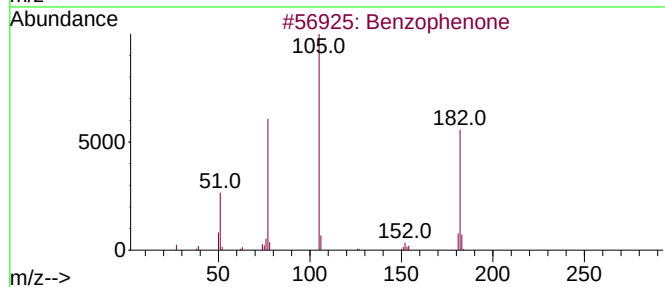
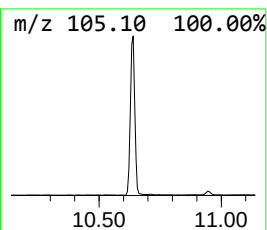
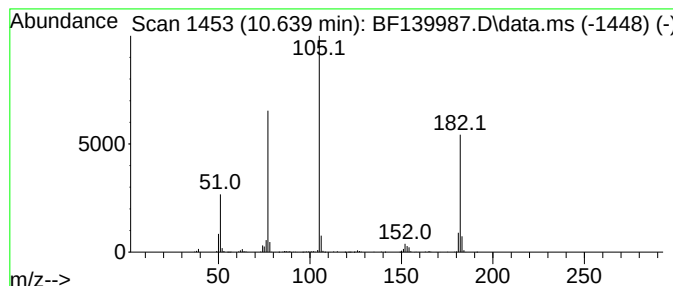
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	12.85 ng	571880	Acenaphthene-d10	9.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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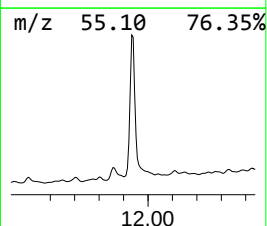
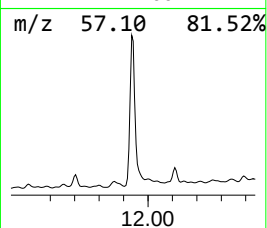
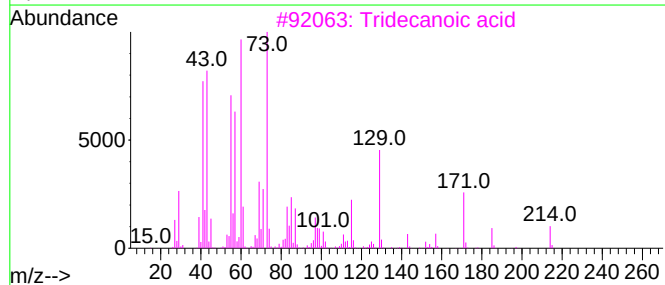
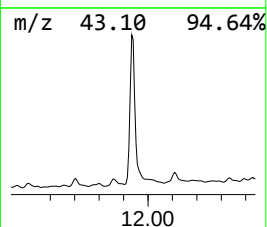
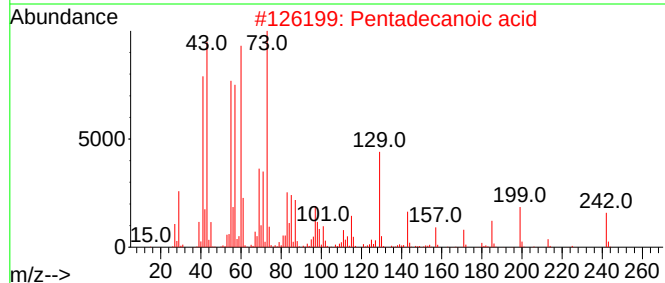
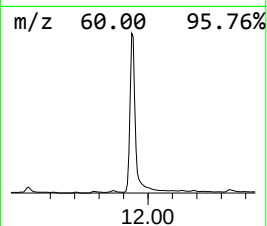
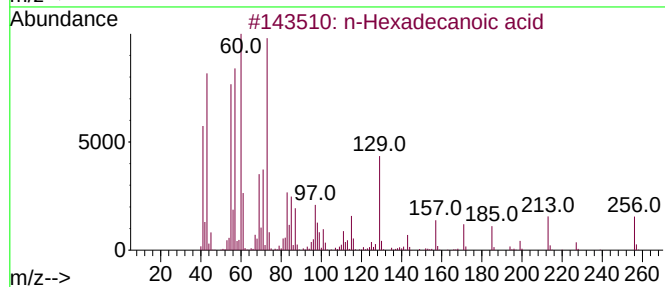
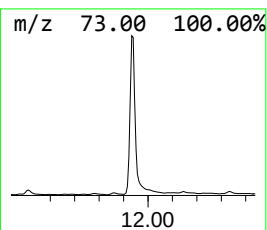
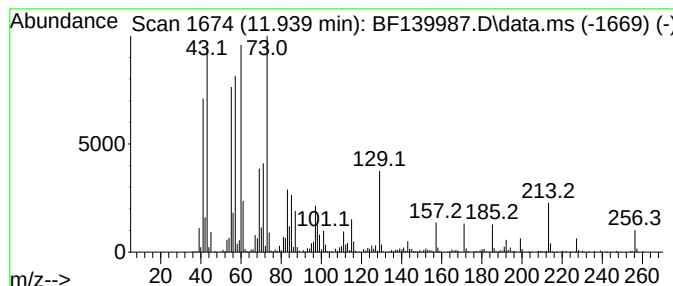
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.939	14.95 ng	760369	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
3	Tridecanoic acid		214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	74
5	Undecanoic acid		186	C11H22O2	000112-37-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139987.D
Acq On : 24 Oct 2024 02:06
Operator : RC/JU
Sample : P4486-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-03-102224

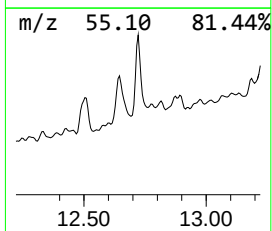
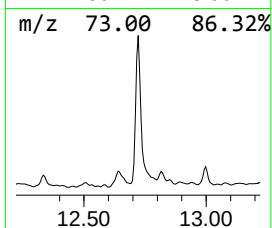
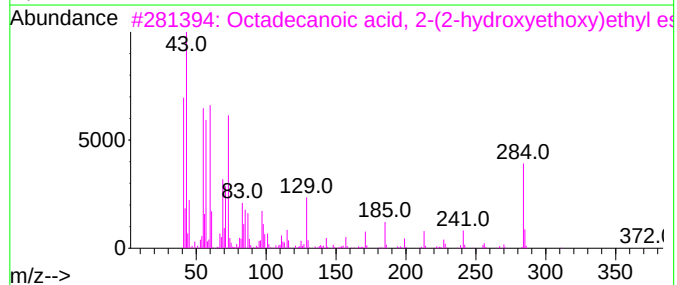
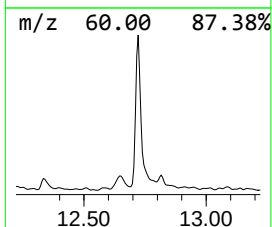
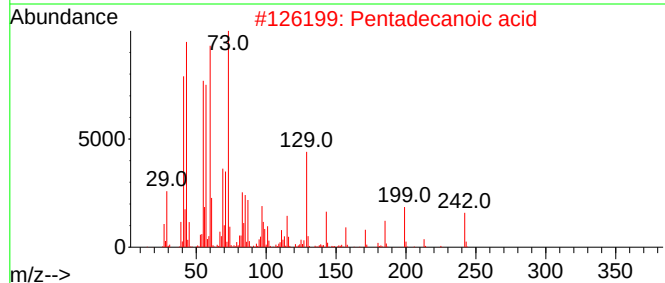
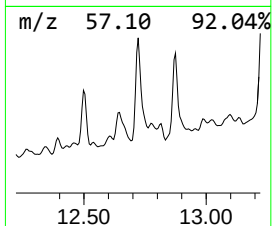
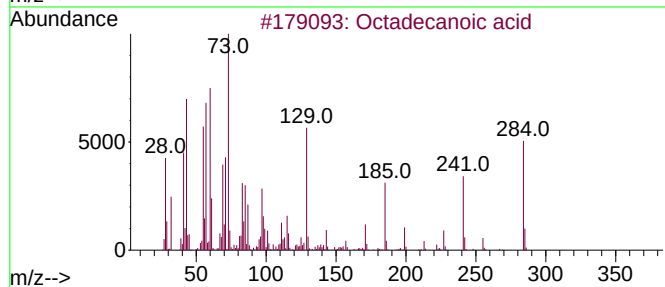
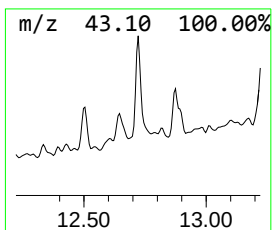
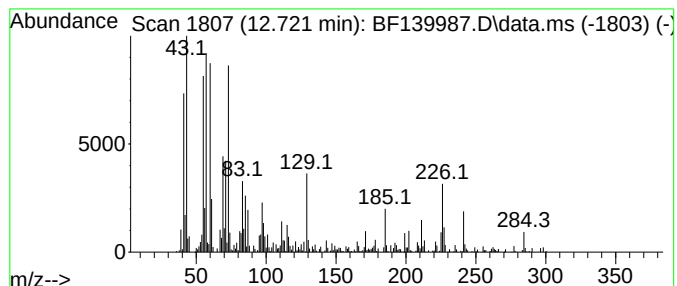
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.721	4.29 ng	217952	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139987.D
Acq On : 24 Oct 2024 02:06
Operator : RC/JU
Sample : P4486-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-03-102224

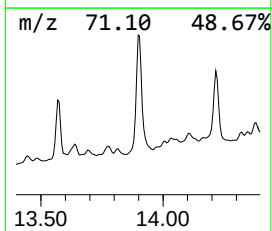
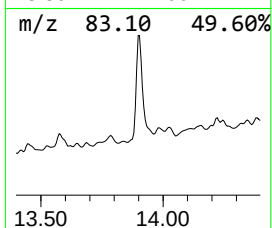
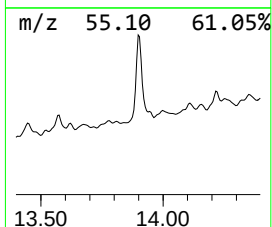
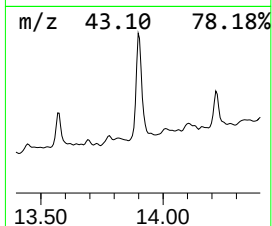
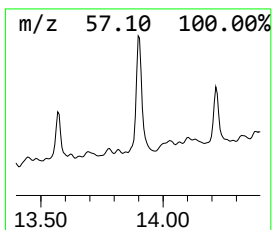
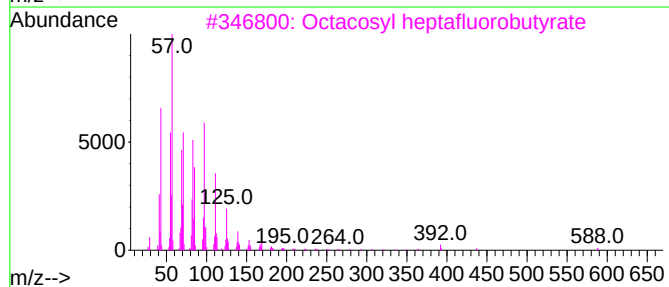
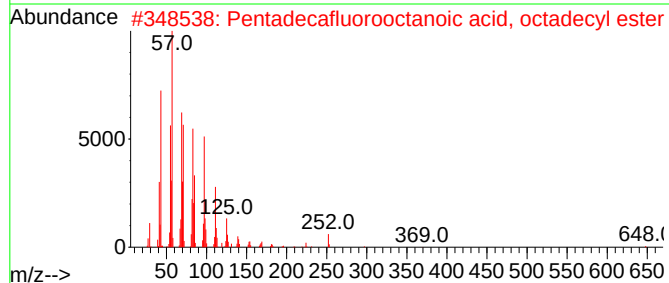
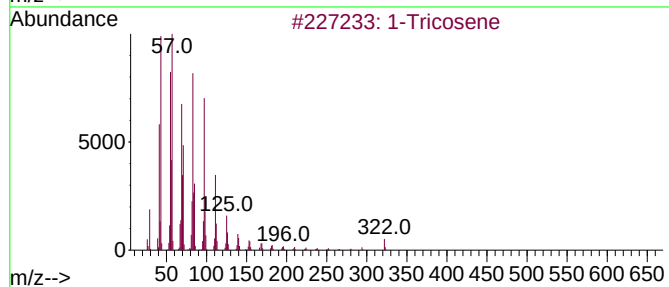
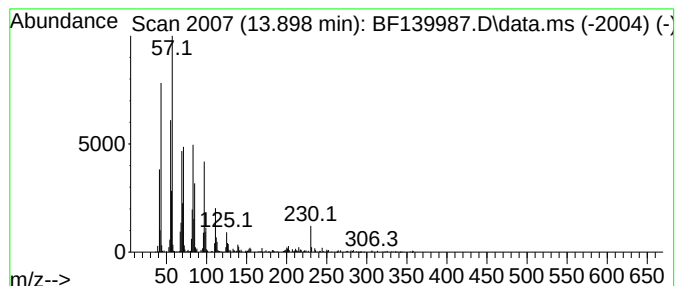
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	8.74 ng	368315	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tricosene	322	C23H46	018835-32-0	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	91
4			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102324\
Data File : BF139987.D
Acq On : 24 Oct 2024 02:06
Operator : RC/JU
Sample : P4486-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-03-102224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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
Butane, 2-metho...	2.181	26.4	ng	1031140	1	6.892	780930	20.0
2-Butenal, 3-me...	5.992	3.5	ng	135045	1	6.892	780930	20.0
Pentanedioic ac...	7.698	2.0	ng	95221	2	8.169	932155	20.0
Benzophenone	10.639	12.9	ng	571880	3	9.927	889968	20.0
n-Hexadecanoic ...	11.939	14.9	ng	760369	4	11.410	1017250	20.0
Octadecanoic acid	12.721	4.3	ng	217952	4	11.410	1017250	20.0
1-Tricosene	13.898	8.7	ng	368315	5	14.051	842688	20.0