

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
 Data File : BF141270.D
 Acq On : 27 Jan 2025 14:11
 Operator : RC/JU
 Sample : Q1187-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-COMP

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: BF141270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	6	13	22	rBV	81539	133148	2.82%	0.422%
2	2.334	32	41	57	rVB	41062	140423	2.97%	0.445%
3	5.022	494	498	509	rVB	47956	77026	1.63%	0.244%
4	5.422	559	566	571	rBV	2770836	3757260	79.50%	11.896%
5	6.434	731	738	743	rBV	2710064	3840086	81.26%	12.158%
6	6.804	796	801	806	rBV	689112	837901	17.73%	2.653%
7	7.363	890	896	901	rBV	1900665	2551268	53.98%	8.078%
8	7.622	935	940	951	rVB	93770	120149	2.54%	0.380%
9	8.087	1013	1019	1024	rBV	859613	1108421	23.45%	3.509%
10	9.163	1196	1202	1207	rBV	3605405	4725932	100.00%	14.963%
11	9.839	1311	1317	1330	rBV	960605	1224522	25.91%	3.877%
12	10.557	1433	1439	1446	rBV	433486	541942	11.47%	1.716%
13	10.628	1446	1451	1466	rBV	1972516	2680098	56.71%	8.486%
14	11.327	1565	1570	1577	rBV	929339	1161045	24.57%	3.676%
15	11.563	1605	1610	1617	rBV2	25415	49669	1.05%	0.157%
16	11.863	1654	1661	1673	rBV	445150	775563	16.41%	2.456%
17	12.116	1699	1704	1712	rVB	60890	84281	1.78%	0.267%
18	12.645	1789	1794	1807	rBV	232716	421928	8.93%	1.336%
19	12.921	1835	1841	1846	rBV	3401044	4524254	95.73%	14.325%
20	13.821	1989	1994	2011	rBV2	128110	277290	5.87%	0.878%
21	13.968	2013	2019	2030	rVB	775666	1106078	23.40%	3.502%
22	14.833	2162	2166	2173	rBV	87061	120557	2.55%	0.382%
23	15.010	2192	2196	2205	rBV	57799	120436	2.55%	0.381%
24	15.310	2243	2247	2252	rVB	36666	56218	1.19%	0.178%
25	15.368	2253	2257	2262	rVV	37584	59073	1.25%	0.187%
26	15.433	2262	2268	2283	rVB	669081	1089355	23.05%	3.449%

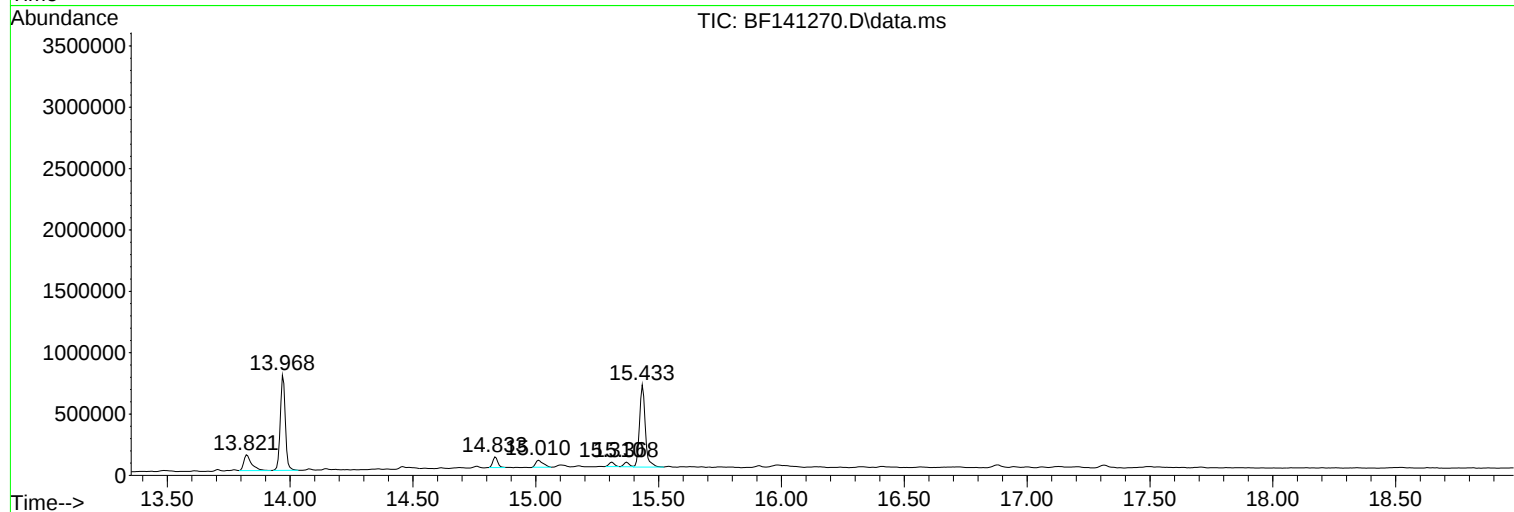
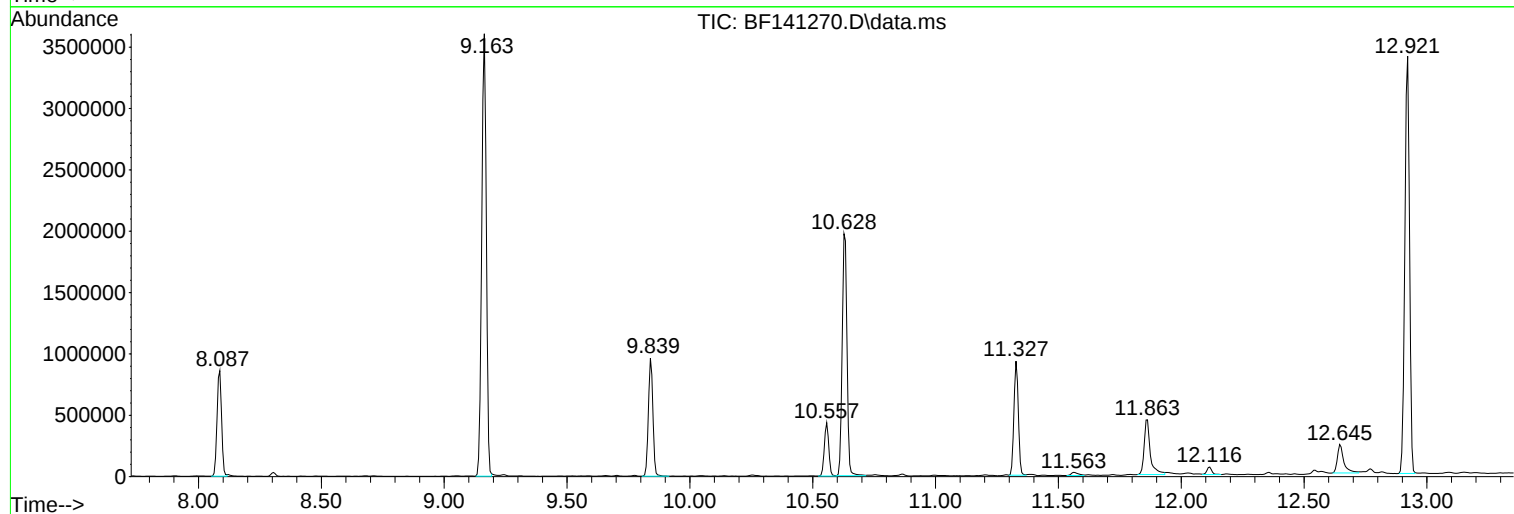
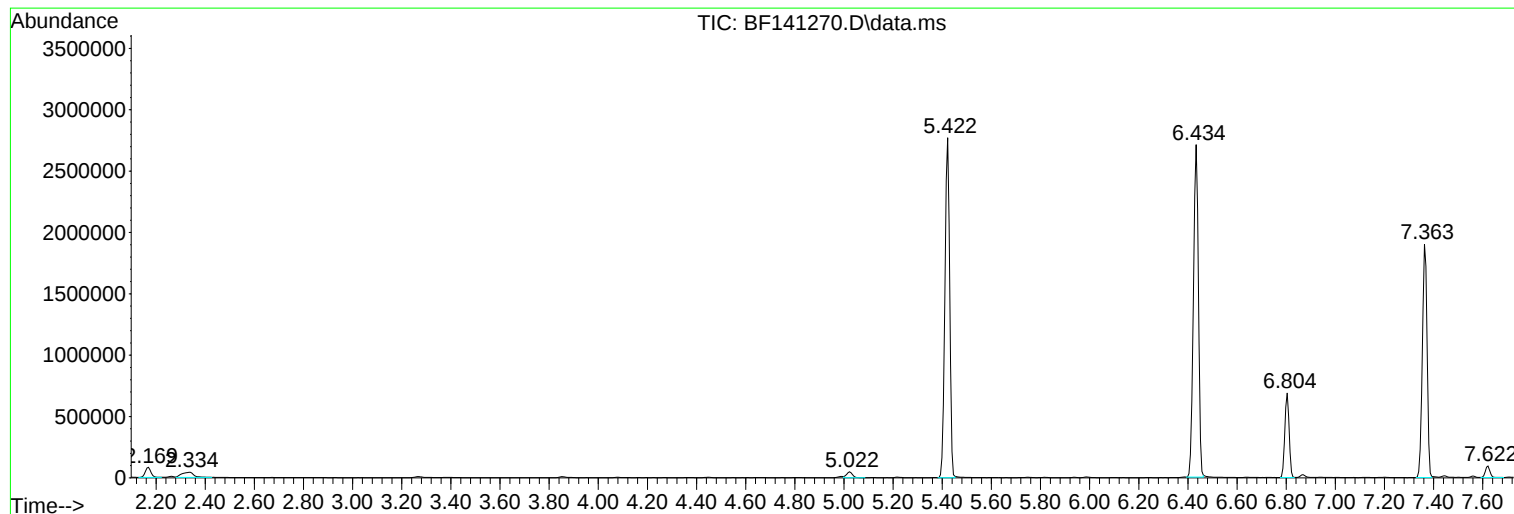
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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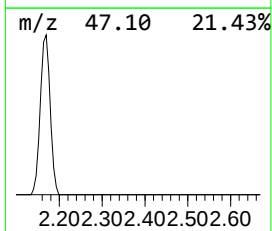
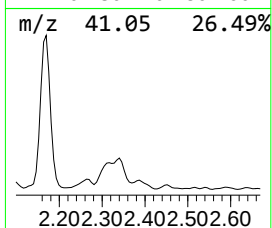
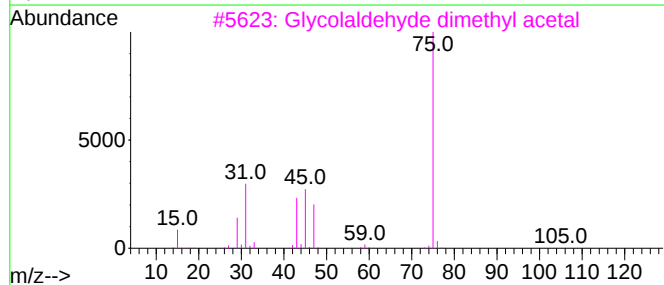
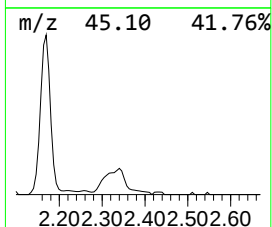
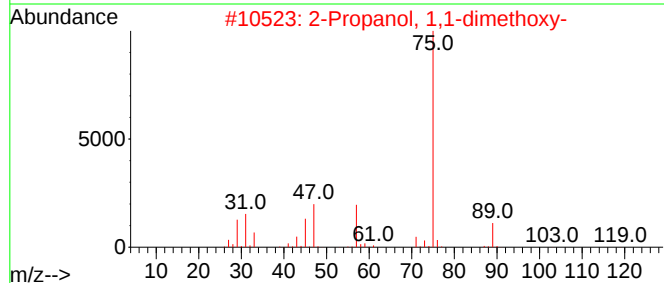
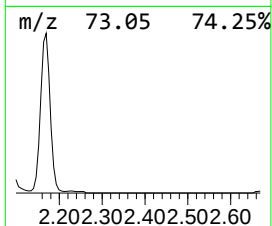
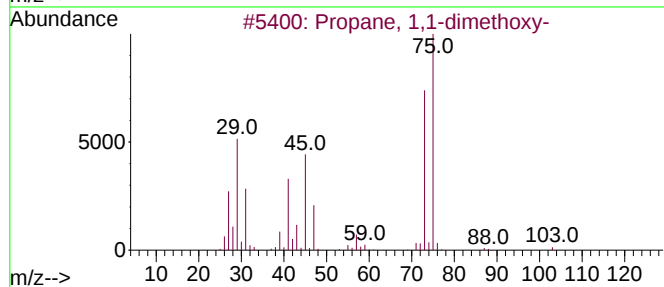
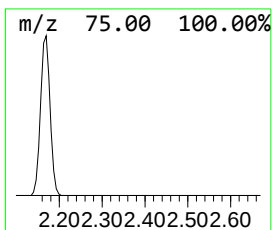
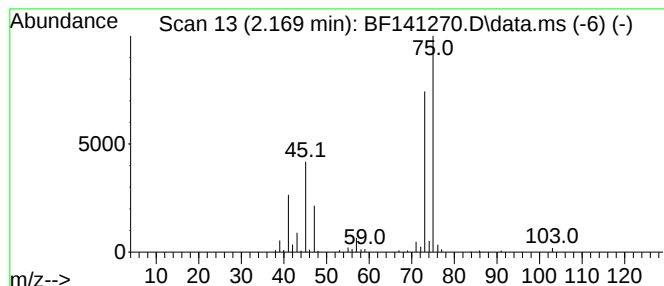
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	3.18 ng	133148	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	40
3			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	36
4			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
5			1-Cyclohexyl-3-ethoxy-butan-2-one	198	C12H22O2	074897-69-1	10



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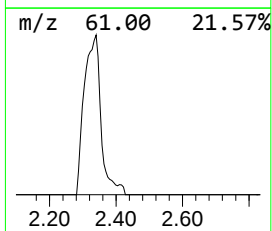
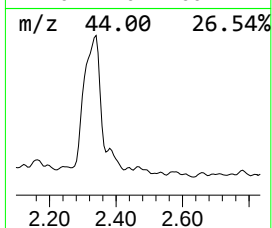
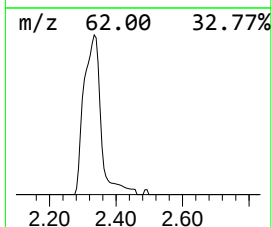
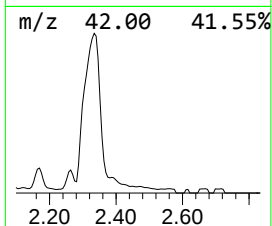
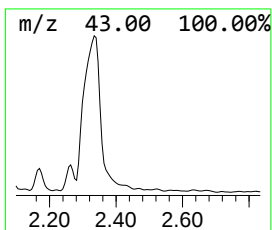
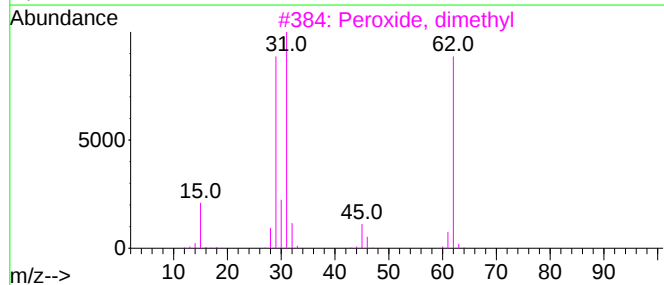
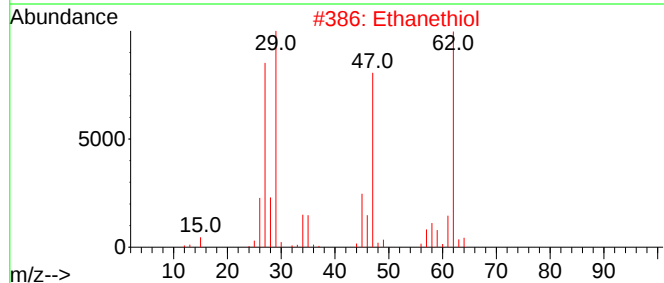
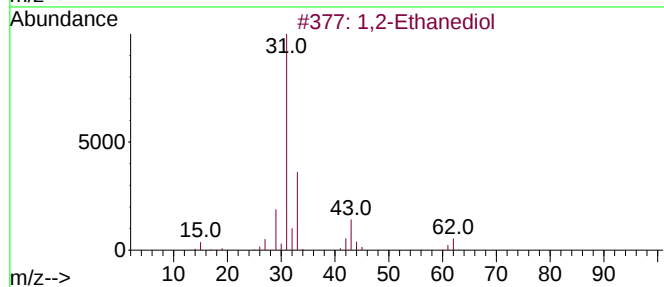
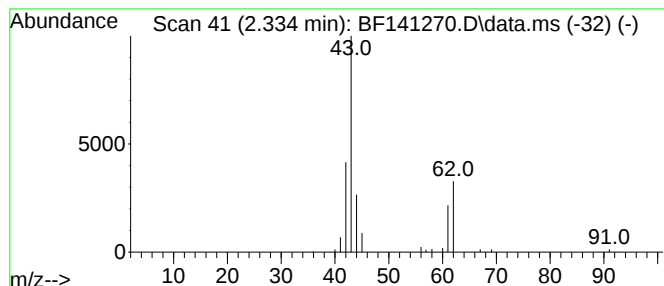
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown2.334 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.334	3.35 ng	140423	1,4-Dichlorobenzene-d4	6.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Ethanediol	62	C2H6O2	000107-21-1	9
2		Ethanethiol	62	C2H6S	000075-08-1	4
3		Peroxide, dimethyl	62	C2H6O2	000690-02-8	4
4		Ethene, chloro-	62	C2H3Cl	000075-01-4	4
5		Monoethanolamine	61	C2H7NO	000141-43-5	3



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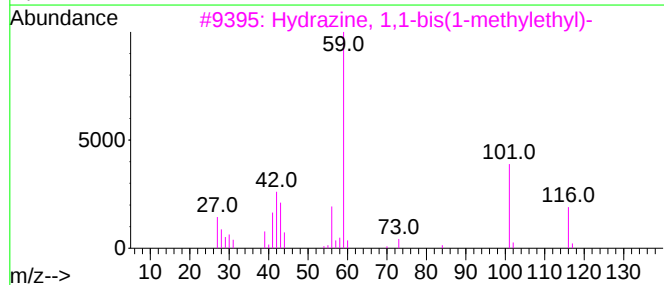
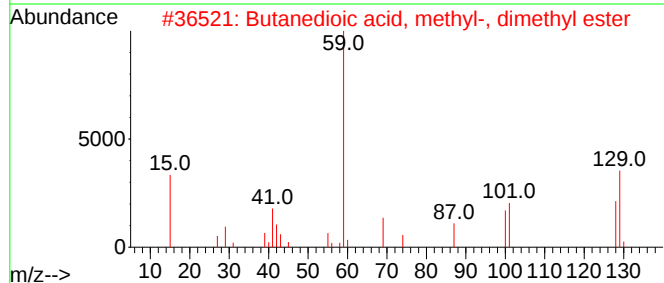
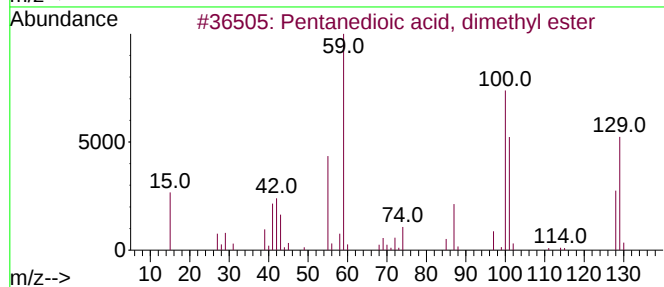
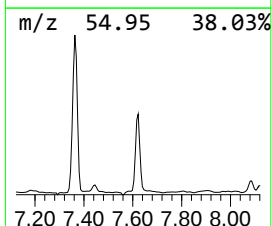
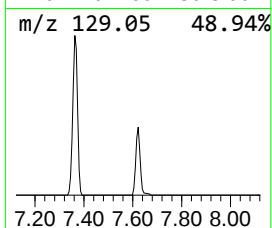
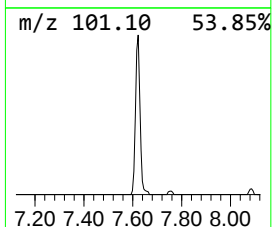
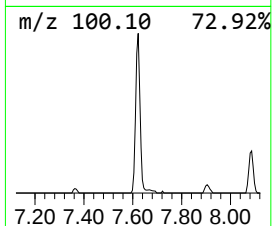
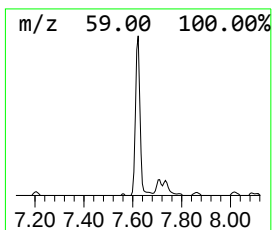
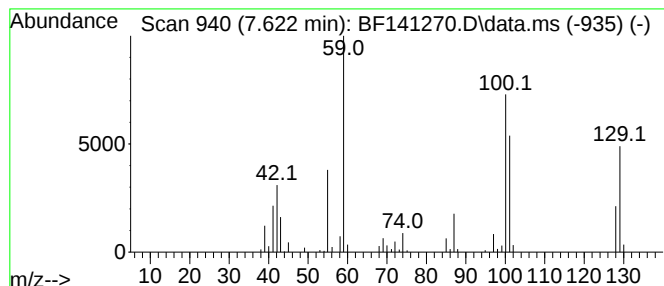
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.622	2.17 ng	120149	Naphthalene-d8	8.086

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	23
4			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	16
5			Oxirane, tetramethyl-	100	C6H12O	005076-20-0	12



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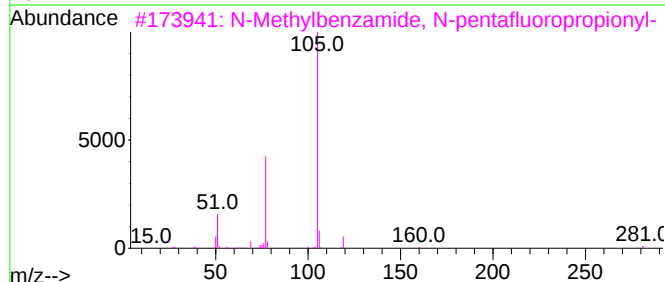
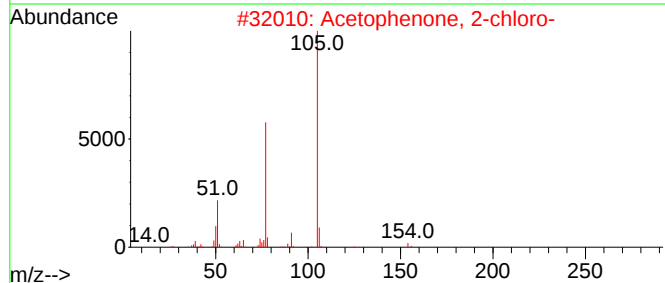
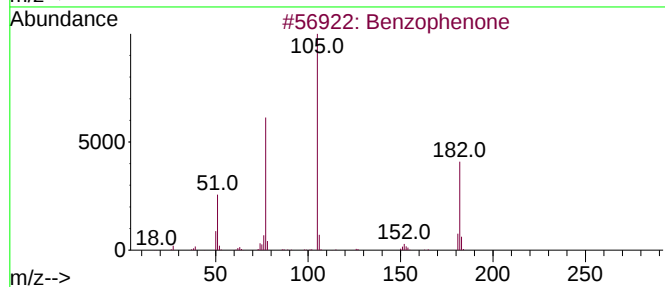
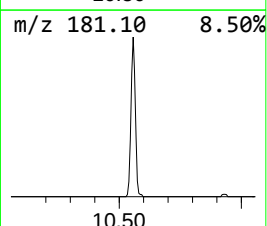
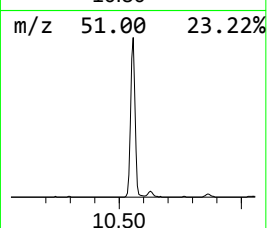
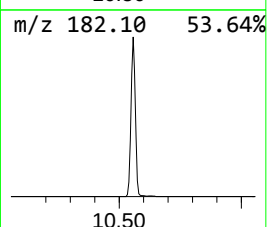
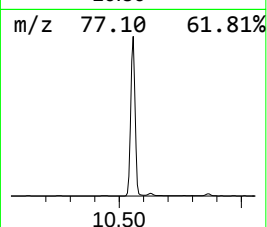
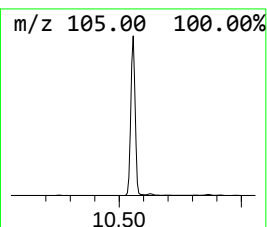
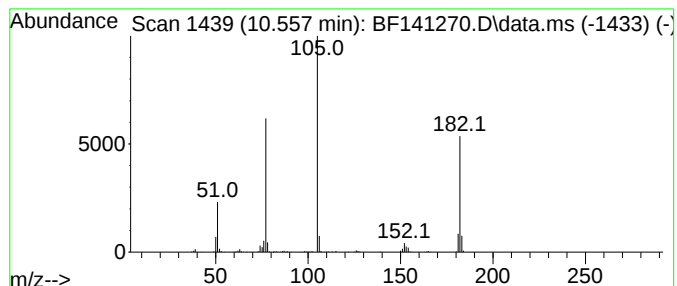
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Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.557	8.85 ng	541942	Acenaphthene-d10	9.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47



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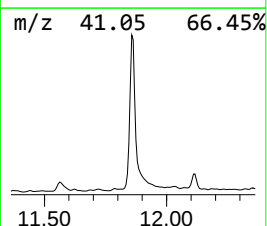
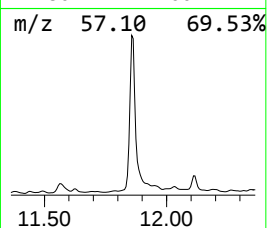
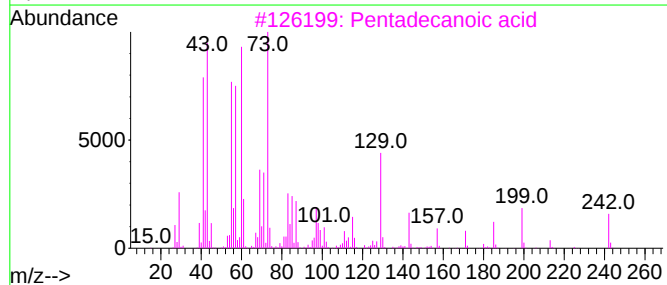
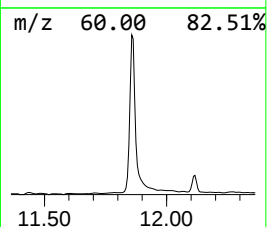
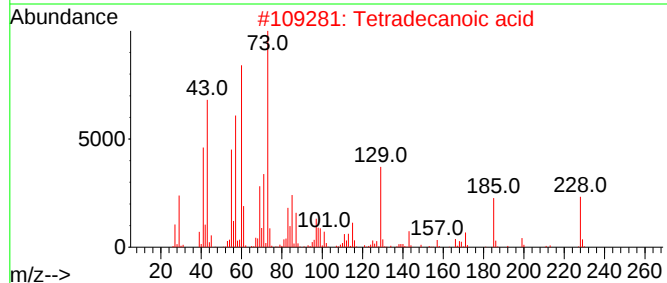
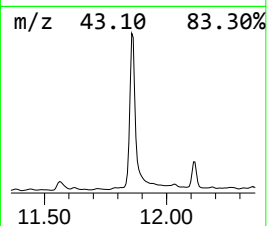
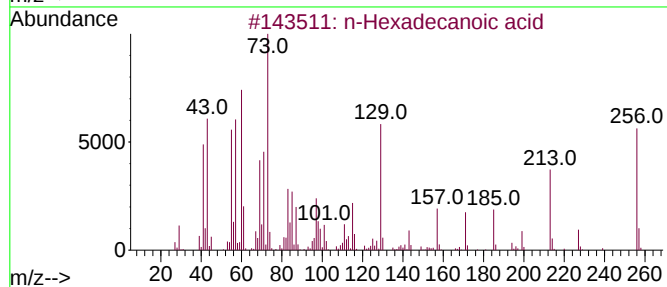
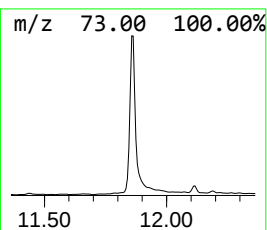
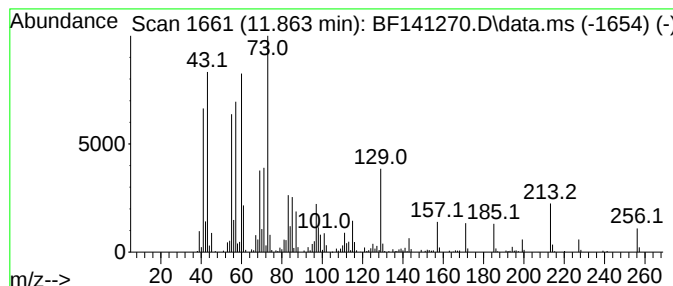
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	13.36 ng	775563	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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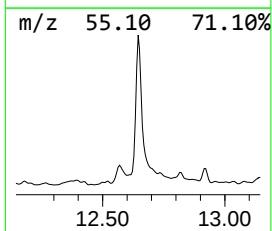
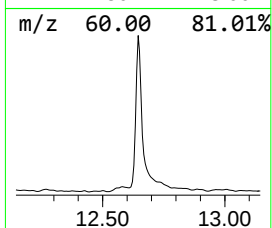
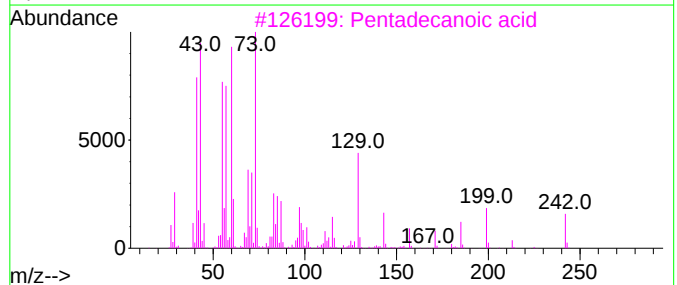
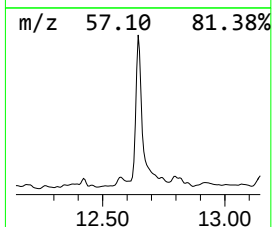
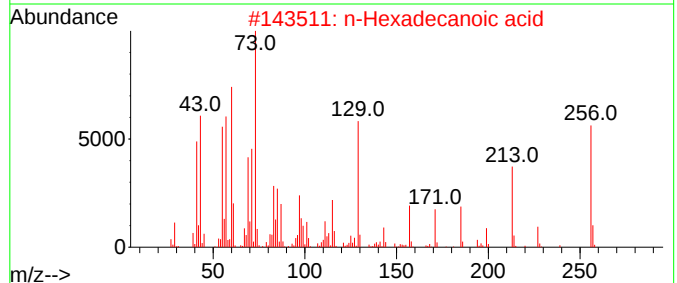
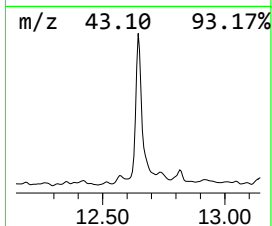
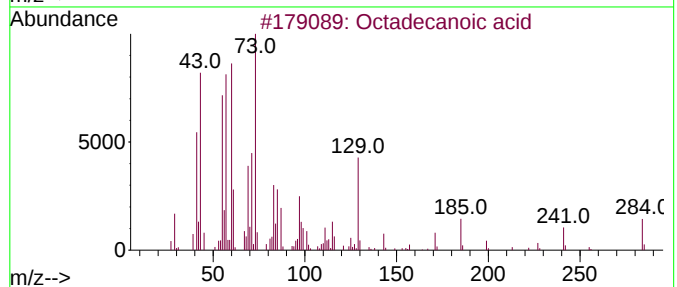
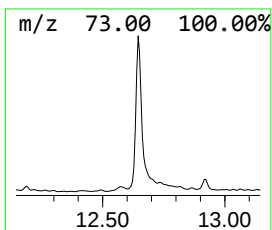
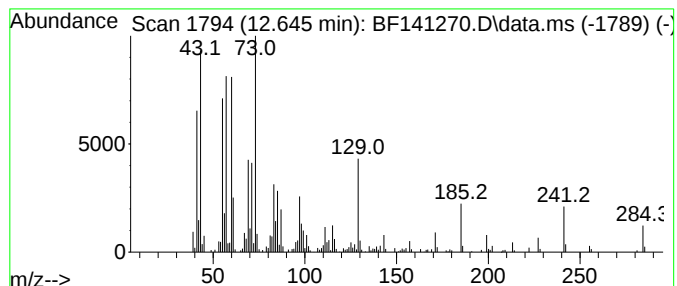
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	7.27 ng	421928	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141270.D
Acq On : 27 Jan 2025 14:11
Operator : RC/JU
Sample : Q1187-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-COMP

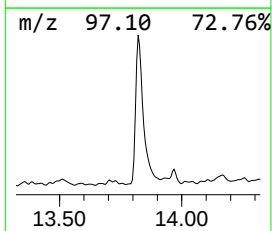
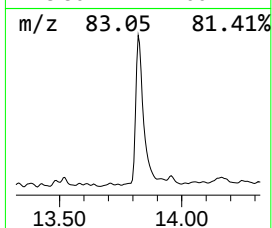
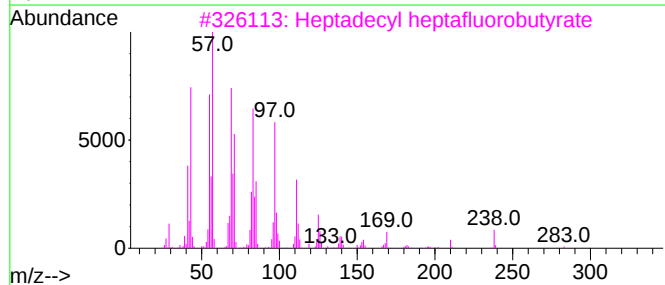
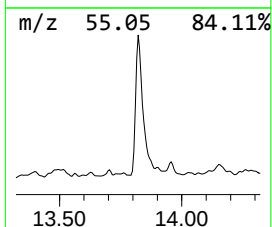
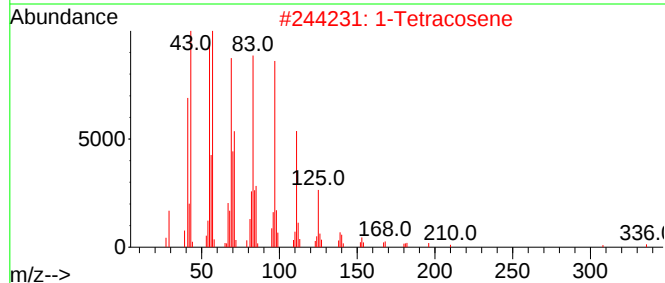
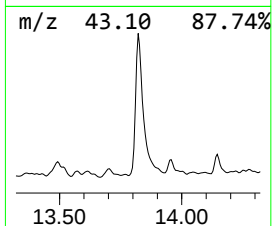
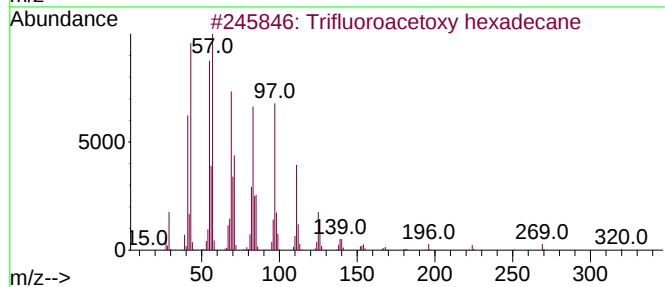
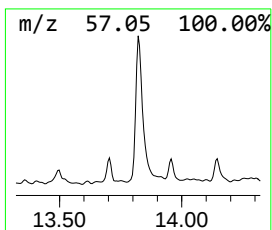
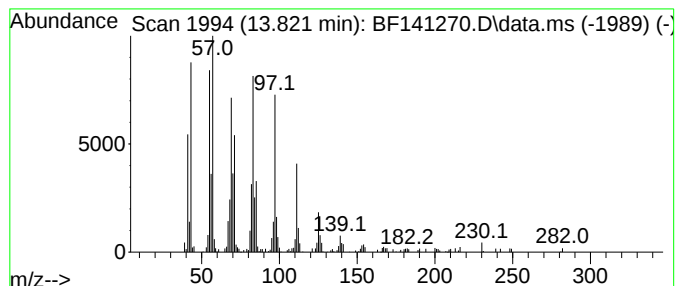
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	5.01 ng	277290	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2			1-Tetracosene	336	C24H48	010192-32-2	95
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141270.D
Acq On : 27 Jan 2025 14:11
Operator : RC/JU
Sample : Q1187-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-COMP

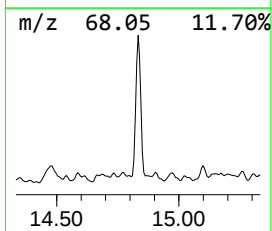
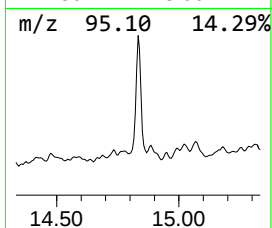
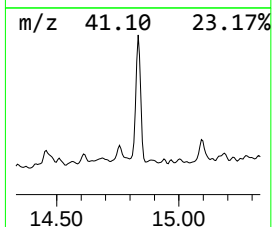
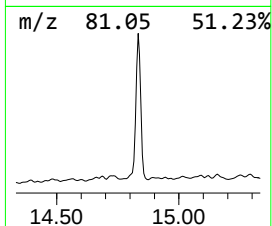
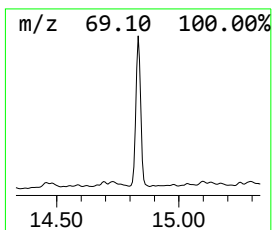
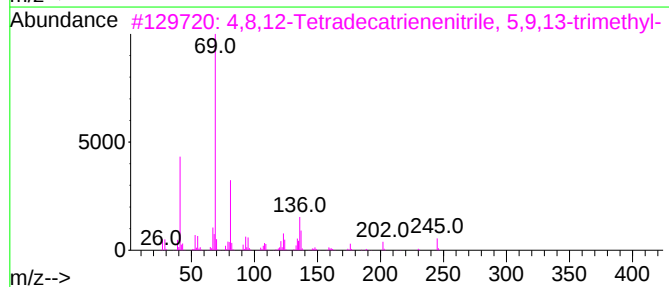
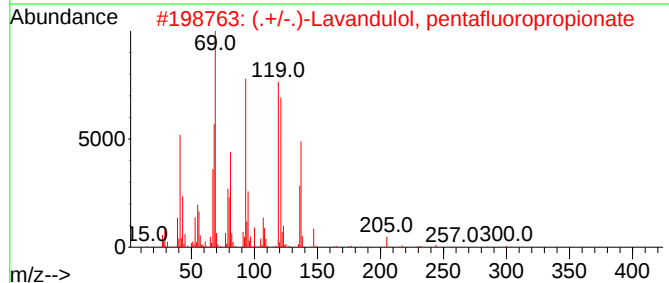
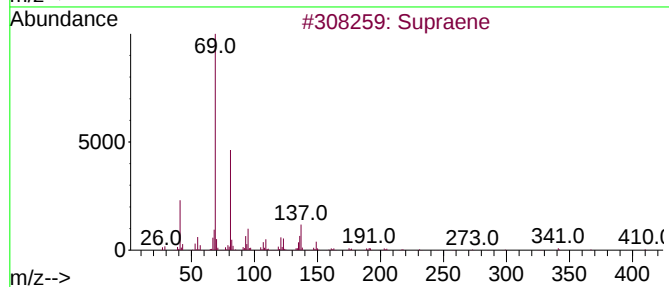
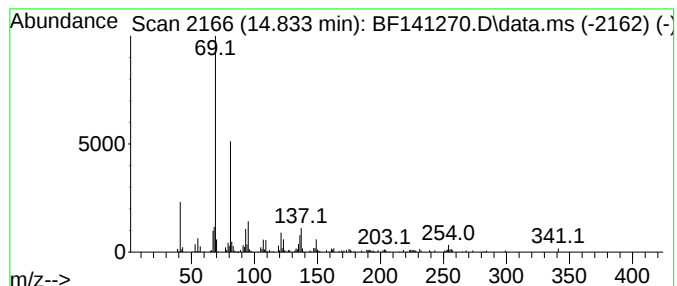
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.21 ng	120557	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
3			4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64
4			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5			trans-Farnesol	222	C15H26O	000106-28-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141270.D
Acq On : 27 Jan 2025 14:11
Operator : RC/JU
Sample : Q1187-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-COMP

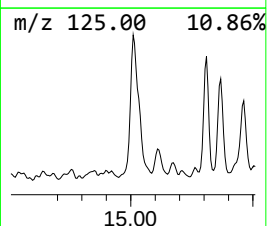
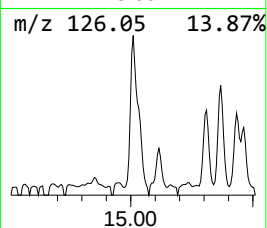
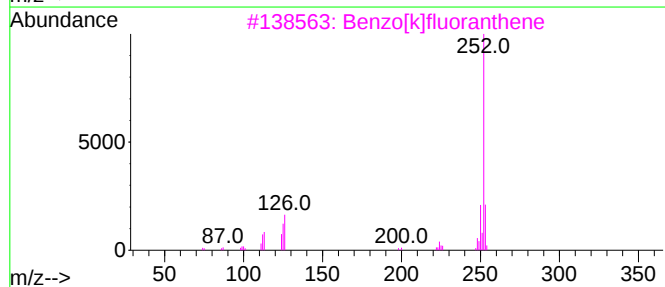
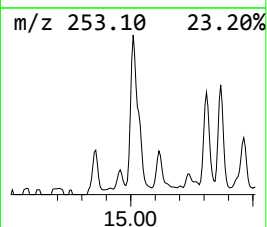
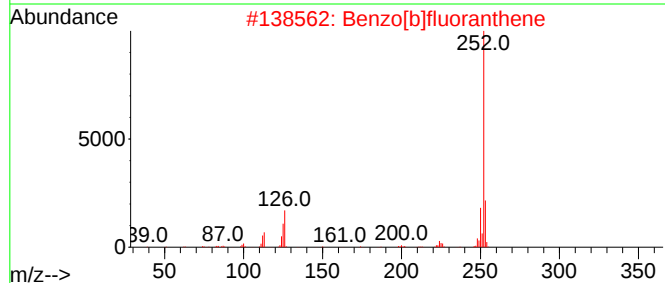
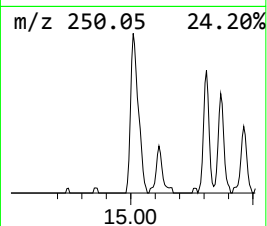
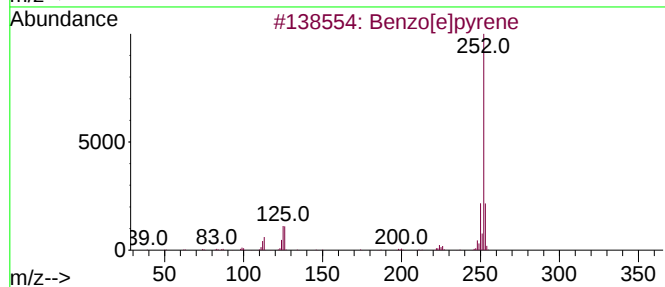
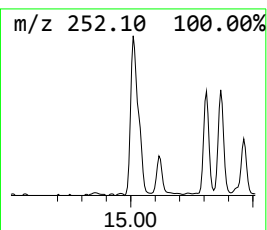
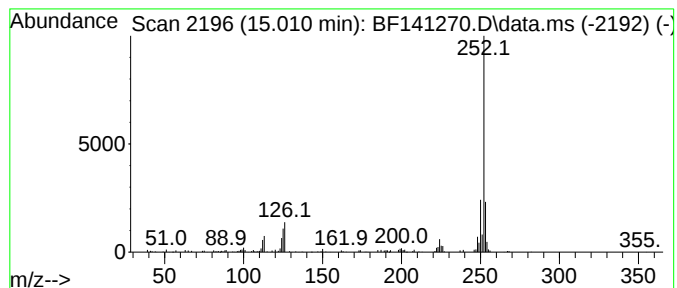
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.010	2.21 ng	120436	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4			Benzo[a]pyrene	252	C20H12	000050-32-8	95
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141270.D
Acq On : 27 Jan 2025 14:11
Operator : RC/JU
Sample : Q1187-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.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
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unknown2.334	2.334	3.4	ng	140423	1	6.804	837901	20.0
Pentanedioic ac...	7.622	2.2	ng	120149	2	8.086	1108420	20.0
Benzophenone	10.557	8.8	ng	541942	3	9.839	1224520	20.0
n-Hexadecanoic ...	11.863	13.4	ng	775563	4	11.328	1161050	20.0
Octadecanoic acid	12.645	7.3	ng	421928	4	11.328	1161050	20.0
Trifluoroacetox...	13.821	5.0	ng	277290	5	13.969	1106080	20.0
Supraene	14.833	2.2	ng	120557	6	15.433	1089360	20.0
Benzo[e]pyrene	15.010	2.2	ng	120436	6	15.433	1089360	20.0