

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
 Data File : BF141769.D
 Acq On : 25 Feb 2025 17:34
 Operator : RC/JU
 Sample : Q1415-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-163-SB01

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-BF020625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141769.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.293	28	34	52	rVB	20550	53463	3.20%	0.412%
2	2.540	69	76	92	rVB	414683	724892	43.36%	5.584%
3	3.216	186	191	220	rBV	37280	118915	7.11%	0.916%
4	4.175	346	354	371	rBV	334532	527025	31.52%	4.060%
5	5.404	558	563	587	rBV	986323	1464643	87.61%	11.283%
6	6.422	731	736	766	rBV	968118	1456506	87.12%	11.220%
7	6.781	792	797	805	rBV	299682	386466	23.12%	2.977%
8	7.345	887	893	906	rBV	645709	928964	55.57%	7.156%
9	7.628	931	941	957	rBV3	11951	38369	2.30%	0.296%
10	8.063	1010	1015	1041	rVB	321653	481091	28.78%	3.706%
11	8.787	1134	1138	1155	rBV	120219	179623	10.74%	1.384%
12	9.134	1192	1197	1208	rBV	1280300	1671850	100.00%	12.879%
13	9.216	1208	1211	1222	rVB	10864	19019	1.14%	0.147%
14	9.816	1307	1313	1327	rBV	333249	477546	28.56%	3.679%
15	10.528	1429	1434	1442	rBV	78466	107009	6.40%	0.824%
16	10.604	1442	1447	1462	rBV	531130	769859	46.05%	5.931%
17	10.851	1479	1489	1495	rBV4	27710	56107	3.36%	0.432%
18	11.151	1535	1540	1551	rBV	17440	30084	1.80%	0.232%
19	11.298	1560	1565	1579	rBV	317303	438056	26.20%	3.375%
20	11.828	1650	1655	1667	rBV2	56818	125203	7.49%	0.965%
21	12.180	1711	1715	1721	rVB	14217	18627	1.11%	0.143%
22	12.622	1785	1790	1797	rBV6	9084	21746	1.30%	0.168%
23	12.686	1797	1801	1807	rVB2	20730	29617	1.77%	0.228%
24	12.880	1829	1834	1845	rBV	1084082	1377952	82.42%	10.615%
25	13.157	1876	1881	1884	rBV	20583	26782	1.60%	0.206%
26	13.416	1921	1925	1928	rBV	14634	19654	1.18%	0.151%
27	13.592	1951	1955	1960	rVB	26004	34299	2.05%	0.264%
28	13.780	1982	1987	2004	rBV4	40646	137269	8.21%	1.057%
29	13.939	2009	2014	2021	rVV	286546	415698	24.86%	3.202%
30	14.004	2021	2025	2032	rVB	28187	44363	2.65%	0.342%
31	14.392	2087	2091	2097	rBV2	33174	54244	3.24%	0.418%
32	14.686	2136	2141	2149	rBV2	95243	153482	9.18%	1.182%
33	14.769	2150	2155	2162	rVB	52048	77876	4.66%	0.600%
34	15.174	2220	2224	2232	rVB3	14604	23937	1.43%	0.184%
35	15.380	2254	2259	2271	rBV	266404	471646	28.21%	3.633%
36	15.815	2330	2333	2339	rVB2	12471	18895	1.13%	0.146%

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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-BF020625.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

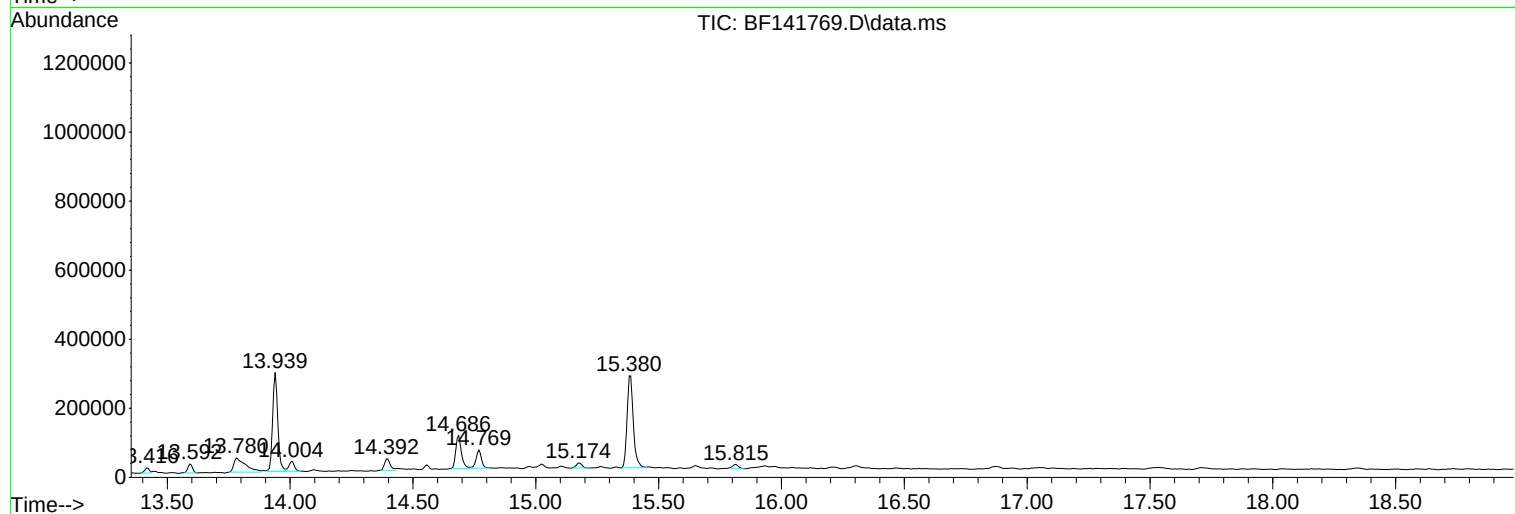
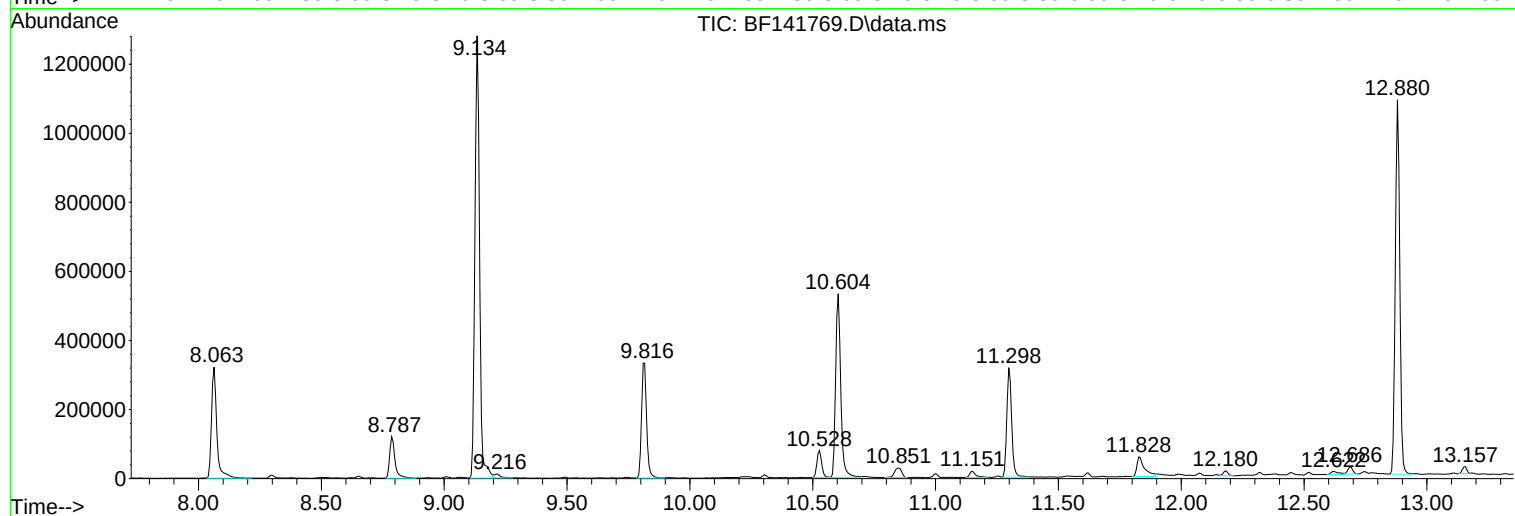
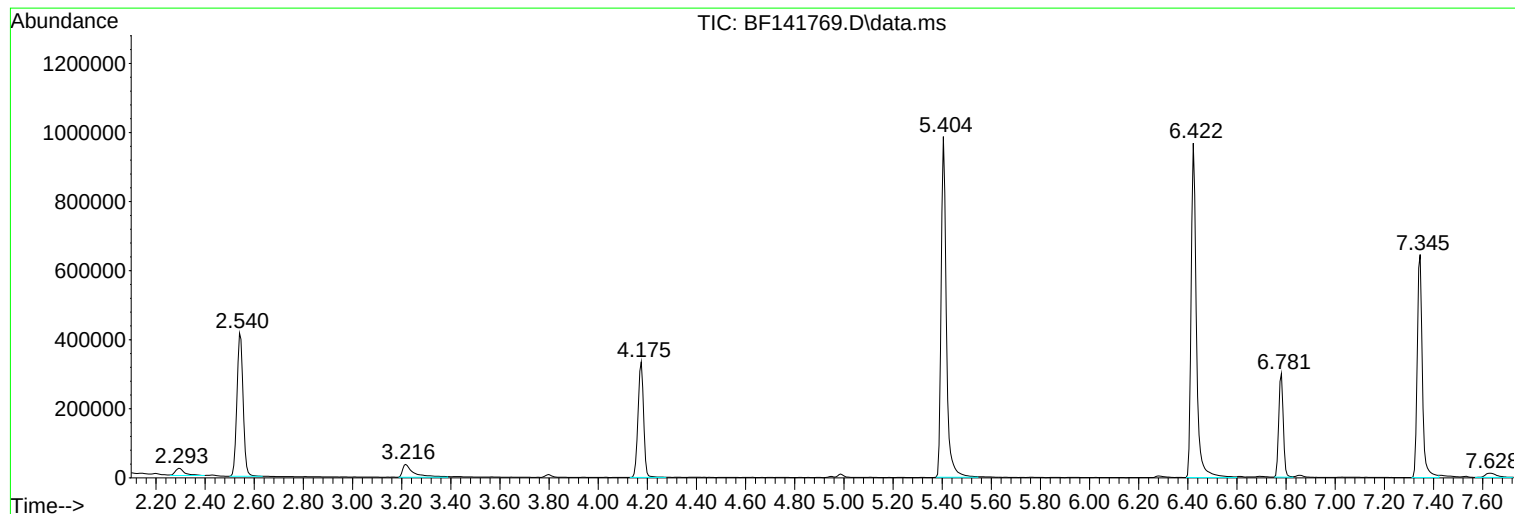
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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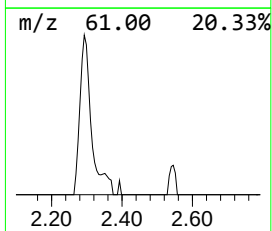
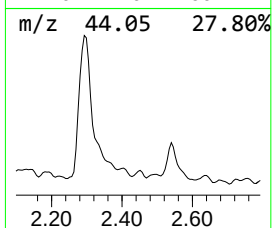
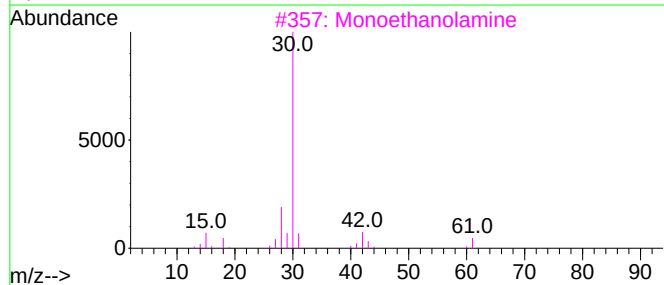
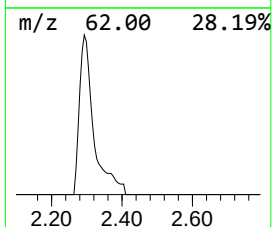
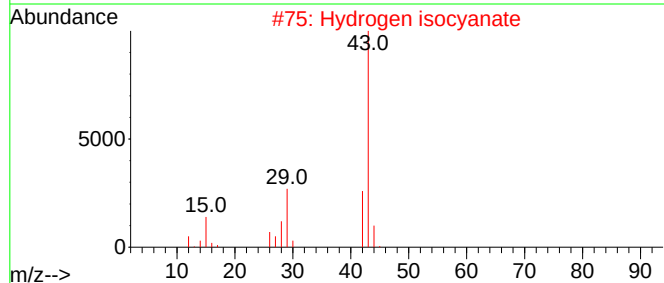
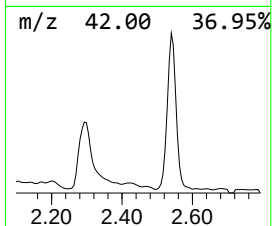
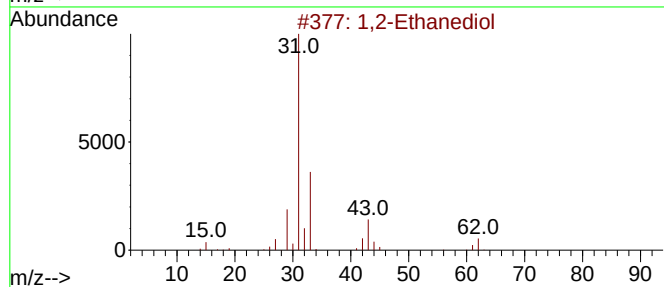
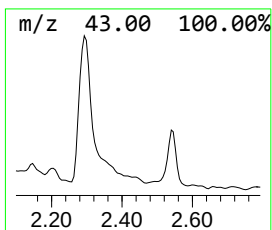
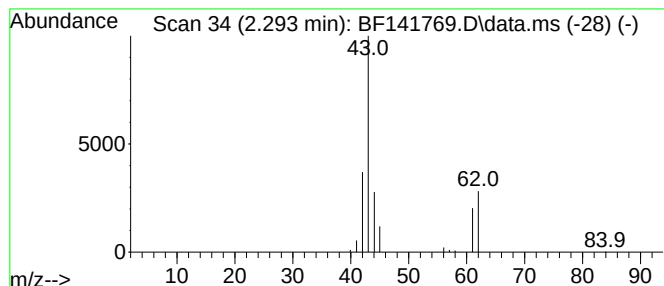
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.293 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.293	2.77 ng	53463	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Ethanediol	62	C2H6O2	000107-21-1	7
2		Hydrogen isocyanate	43	CHNO	000075-13-8	3
3		Monoethanolamine	61	C2H7NO	000141-43-5	3
4		Peroxide, dimethyl	62	C2H6O2	000690-02-8	3
5		n-Propyl fluoride	62	C3H7F	000460-13-9	3



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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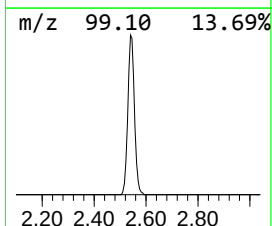
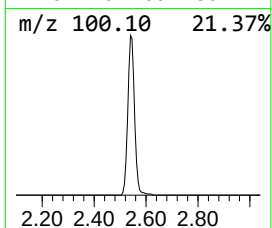
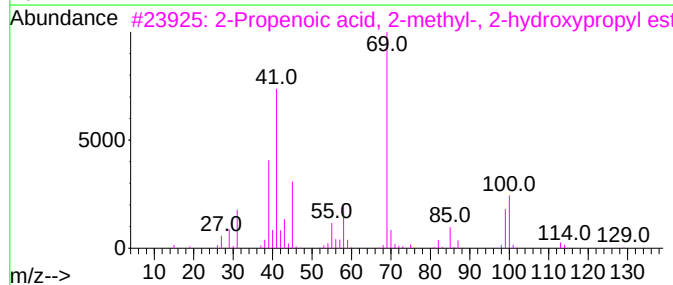
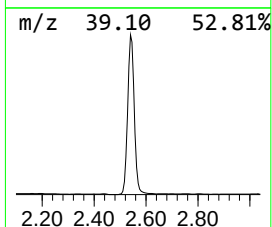
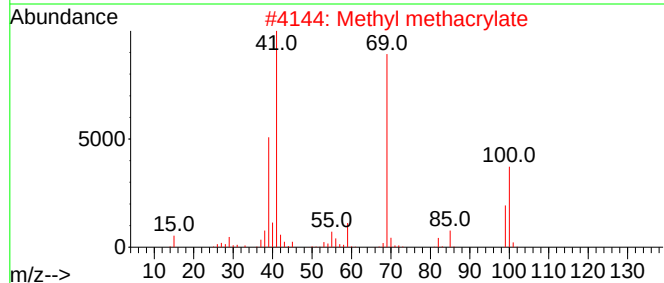
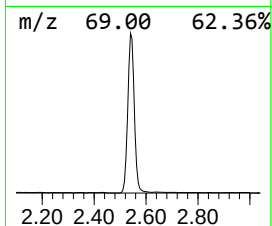
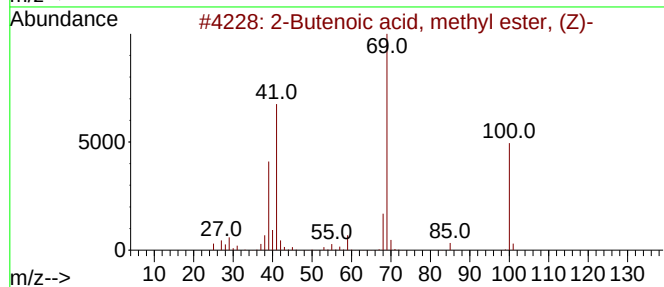
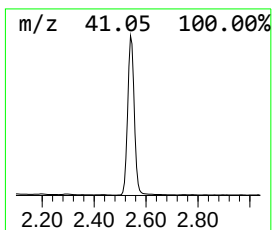
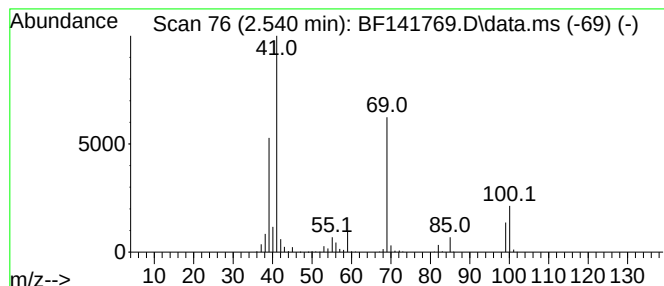
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Butenoic acid, methyl est... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.540	37.51 ng	724892	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenoic acid, methyl ester, (Z)-	100	C5H8O2	004358-59-2	80
2			Methyl methacrylate	100	C5H8O2	000080-62-6	64
3			2-Propenoic acid, 2-methyl-, 2-h...	144	C7H12O3	000923-26-2	56
4			2-Butenoic acid, methyl ester, (E)-	100	C5H8O2	000623-43-8	47
5			2-Propenoic acid, 2-methyl-, 2-p...	124	C7H8O2	013861-22-8	32



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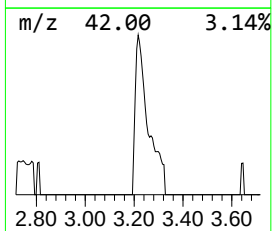
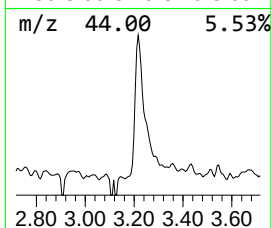
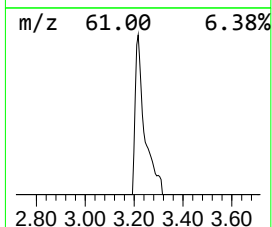
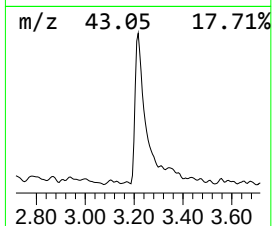
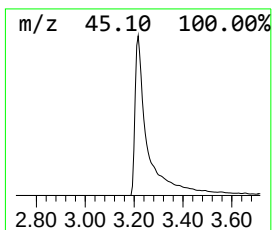
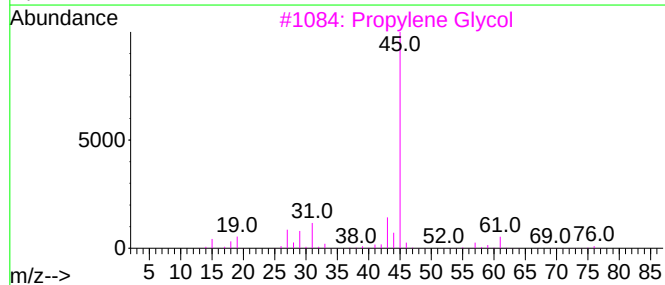
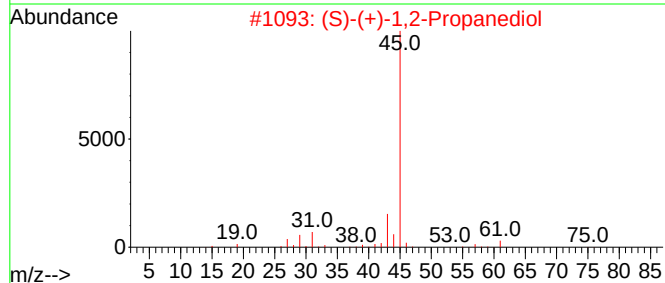
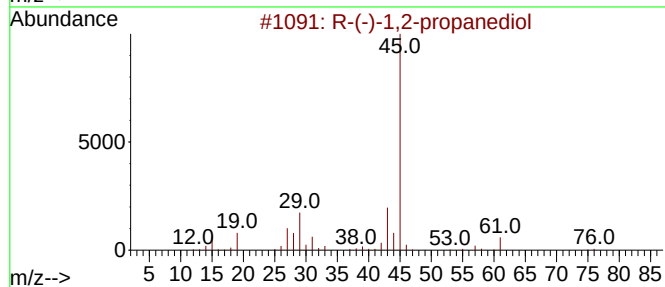
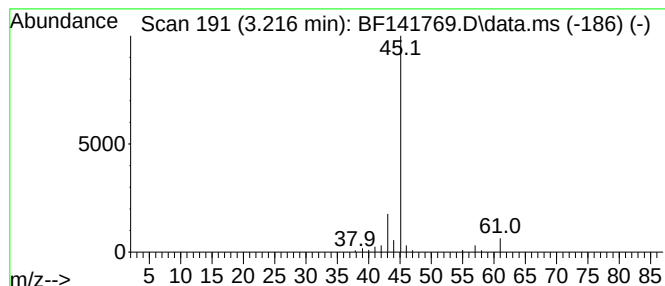
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown3.216 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.216	6.15 ng	118915	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
2	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	9
3	Propylene Glycol			76	C3H8O2	000057-55-6	9
4	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	9
5	L-Lactic acid			90	C3H6O3	000079-33-4	9



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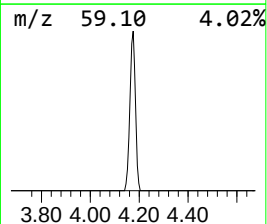
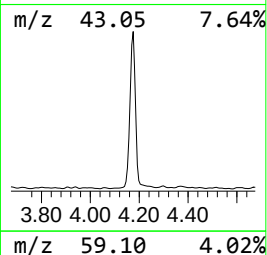
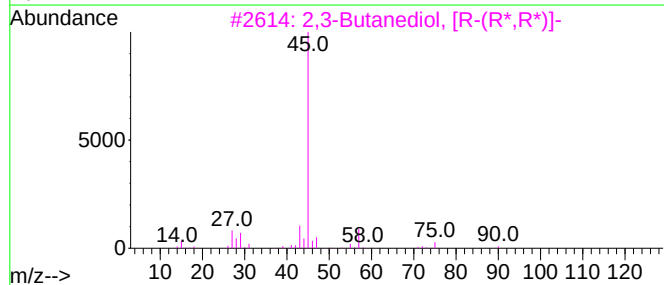
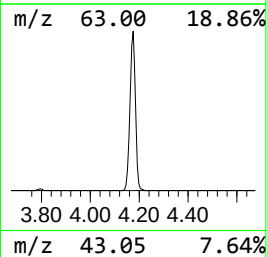
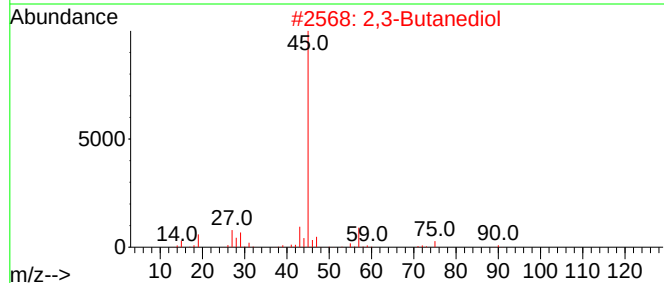
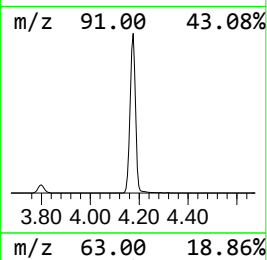
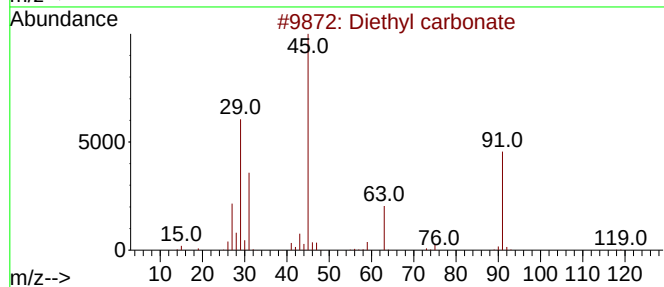
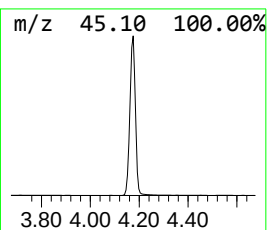
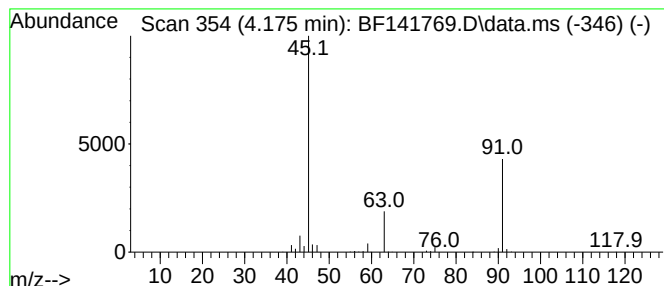
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Diethyl carbonate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.175	27.27 ng	527025	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyl carbonate	118	C5H10O3	000105-58-8	83
2			2,3-Butanediol	90	C4H10O2	000513-85-9	36
3			2,3-Butanediol, [R-(R*,R*)]-	90	C4H10O2	024347-58-8	9
4			Diethyl pyrocarbonate	162	C6H10O5	001609-47-8	9
5			Butane, 1-methoxy-	88	C5H12O	000628-28-4	9



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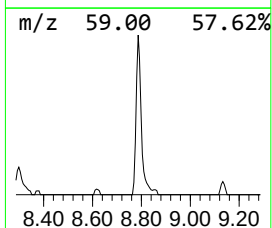
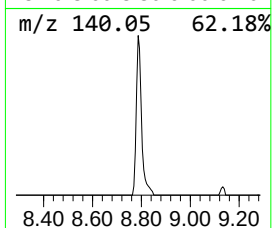
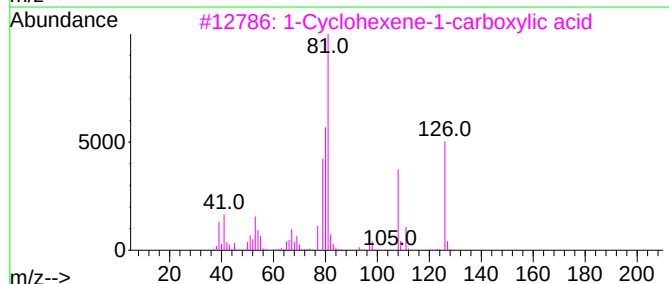
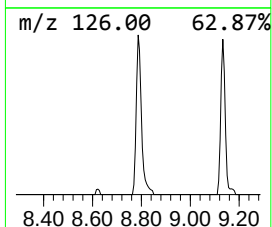
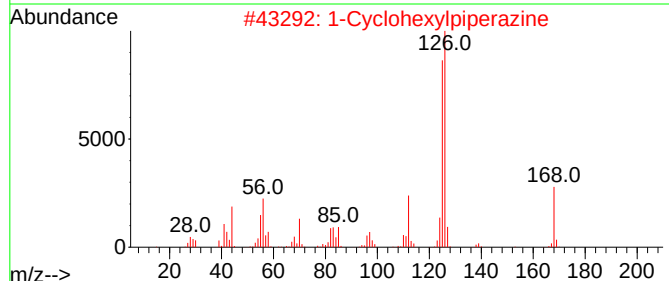
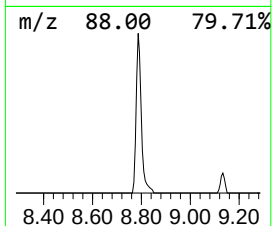
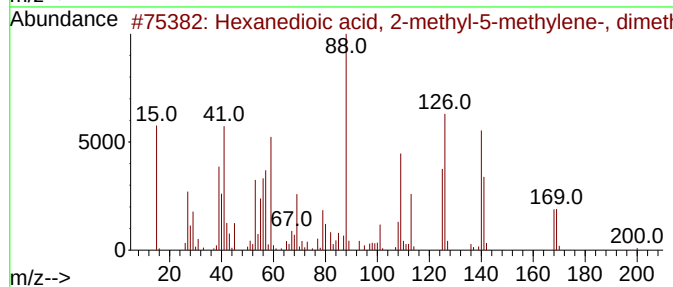
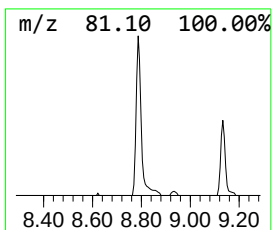
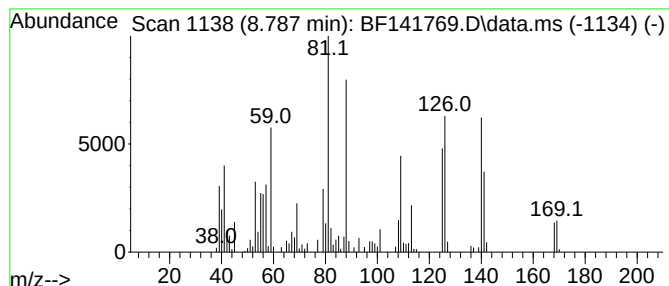
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Peak Number 5 Hexanedioic acid, 2-methyl-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	7.47 ng	179623	Naphthalene-d8	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, 2-methyl-5-met...	200	C10H16O4	004513-62-6	58
2			1-Cyclohexylpiperazine	168	C10H20N2	1000484-48-8	15
3			1-Cyclohexene-1-carboxylic acid	126	C7H10O2	000636-82-8	14
4			1-Chlorosulfonyl-3-methyl-1-azas...	251	C9H14ClNO3S	016933-89-4	14
5			1-(4-Methylhexahydrocyclopenta[b...	182	C11H18O2	1000186-82-3	14



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Acq On : 25 Feb 2025 17:34
Operator : RC/JU
Sample : Q1415-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-163-SB01

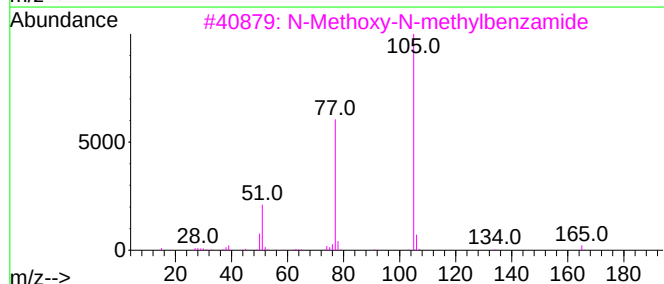
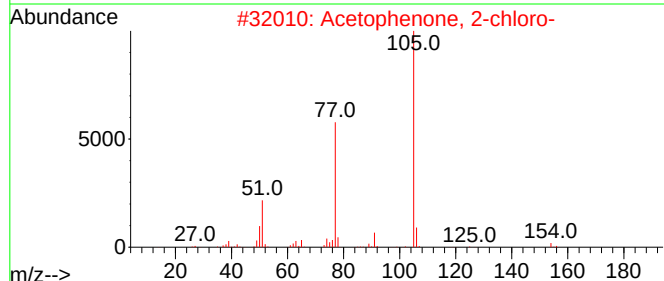
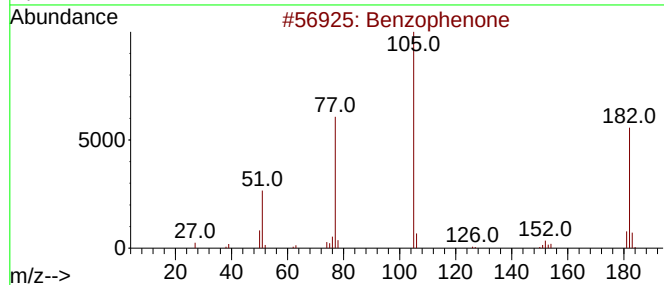
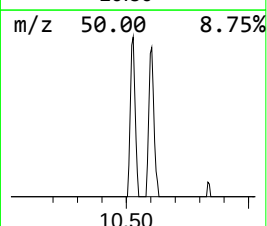
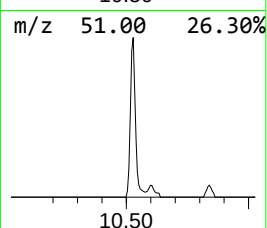
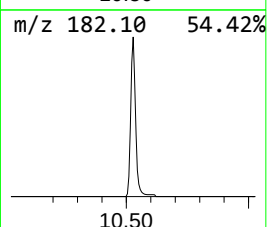
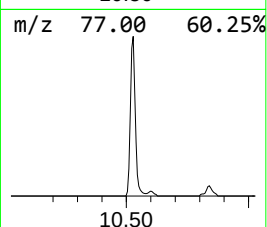
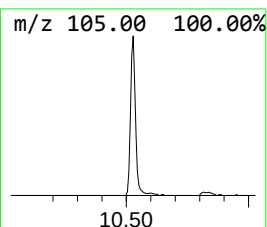
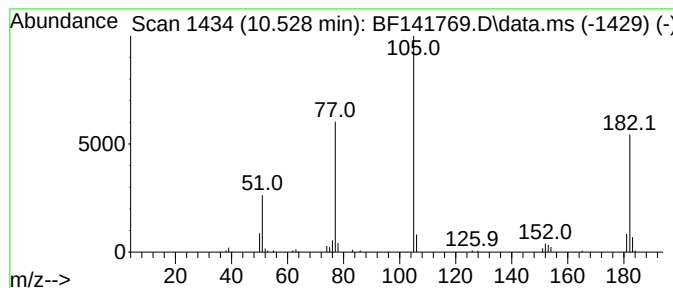
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.528	4.48 ng	107009	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141769.D
Acq On : 25 Feb 2025 17:34
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Sample : Q1415-01
Misc :
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Instrument :
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ClientSampleId :
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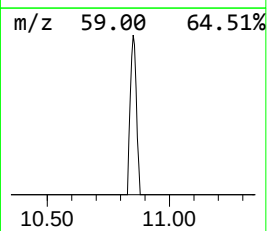
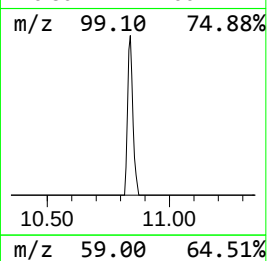
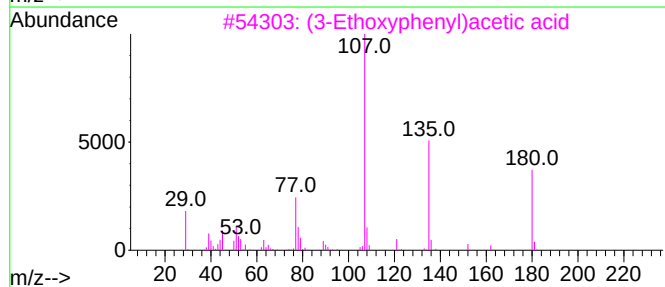
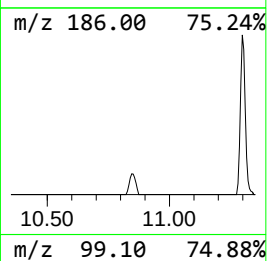
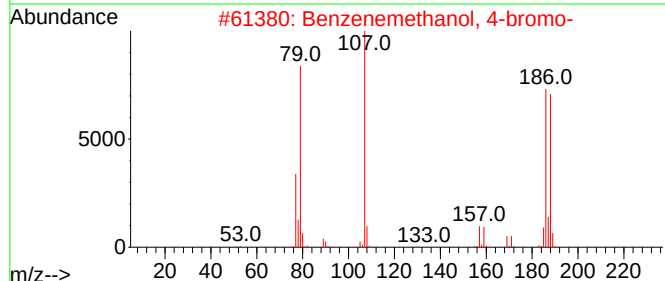
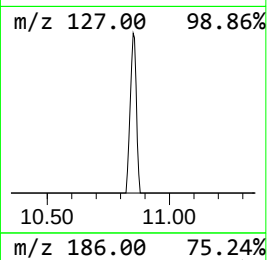
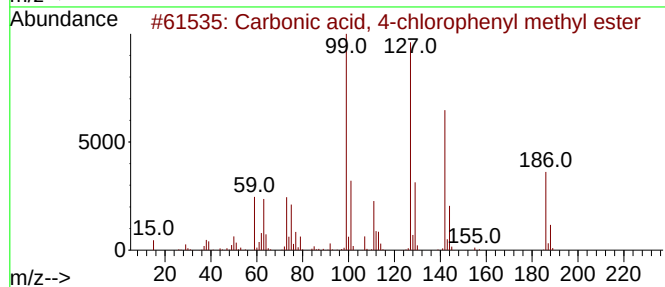
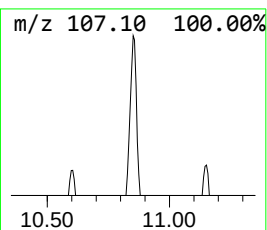
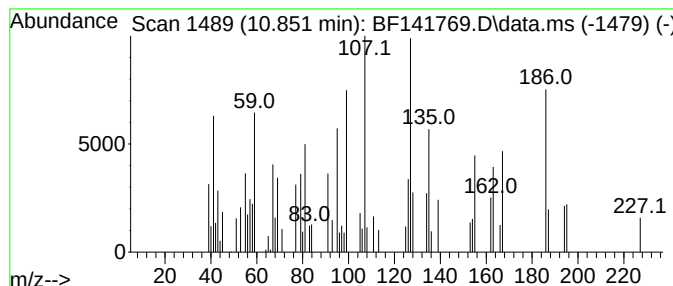
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown10.851 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	2.56 ng	56107	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, 4-chlorophenyl me...	186	C8H7ClO3	024260-28-4	35
2			Benzenemethanol, 4-bromo-	186	C7H7BrO	000873-75-6	10
3			(3-Ethoxyphenyl)acetic acid	180	C10H12O3	072775-83-8	10
4			Ethyl propylphosphonofluoridate	154	C5H12F02P	1000298-31-3	10
5			1,3-Cyclopentadiene, 1,3-bis(1-m...	150	C11H18	123278-27-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141769.D
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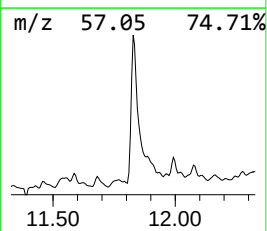
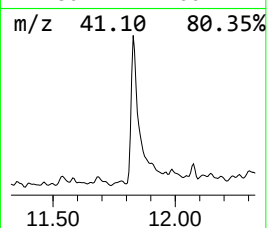
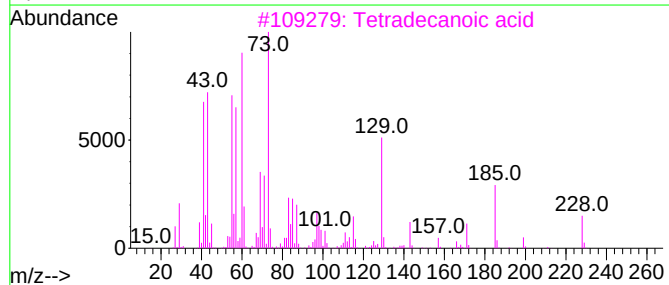
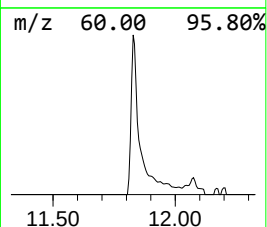
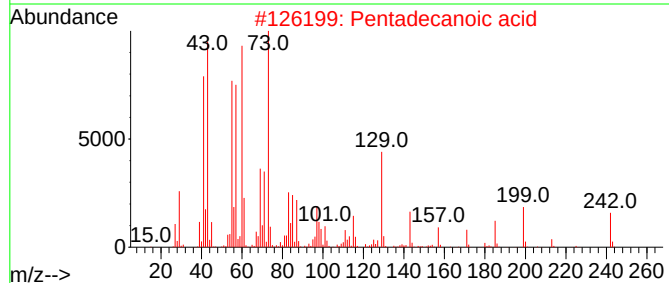
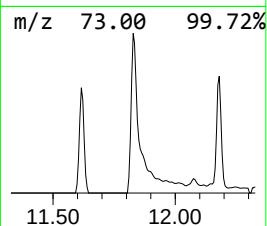
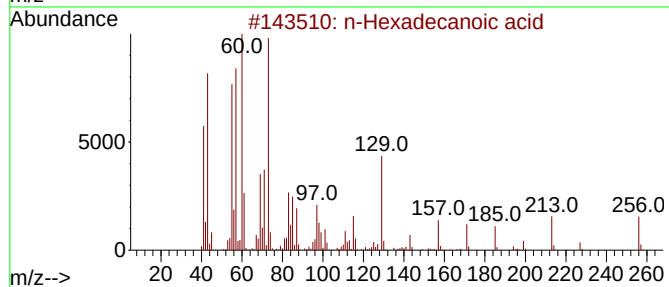
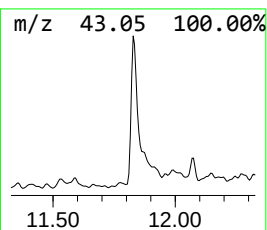
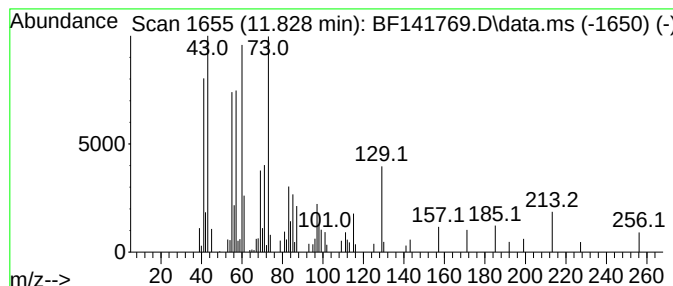
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.828	5.72 ng	125203	Phenanthrene-d10		11.298	
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	90
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	87
4	Tridecanoic acid		214	C13H26O2	000638-53-9	86
5	Oxalic acid, allyl octadecyl ester		382	C23H42O4	1000309-24-5	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141769.D
Acq On : 25 Feb 2025 17:34
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Sample : Q1415-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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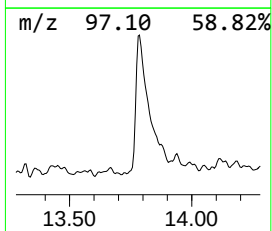
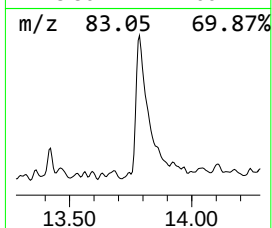
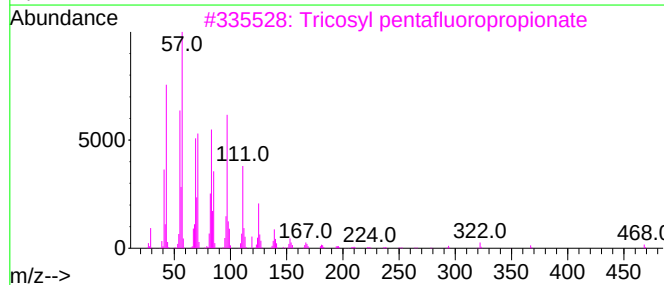
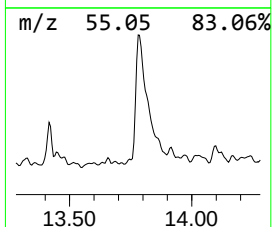
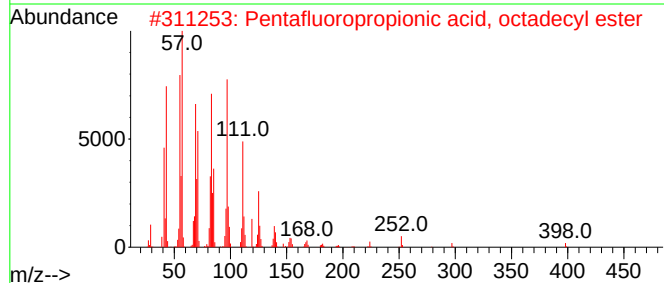
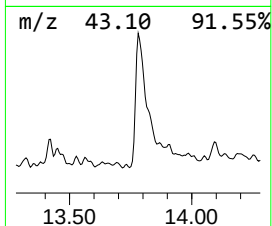
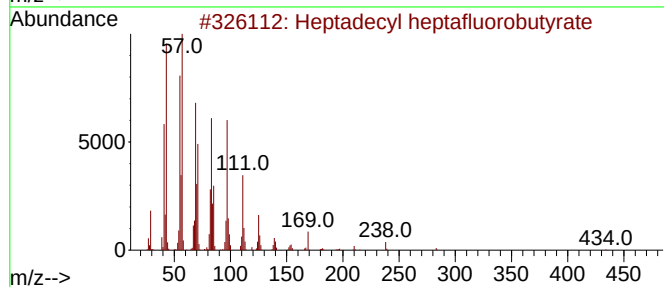
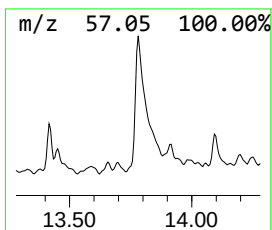
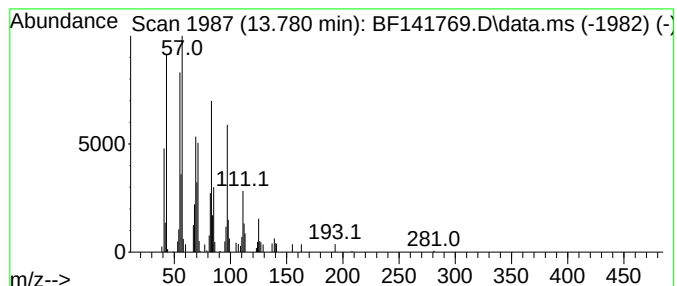
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	6.60 ng	137269	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
3			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
4			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5			Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141769.D
Acq On : 25 Feb 2025 17:34
Operator : RC/JU
Sample : Q1415-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B-163-SB01

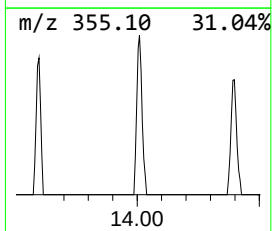
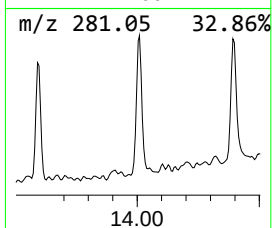
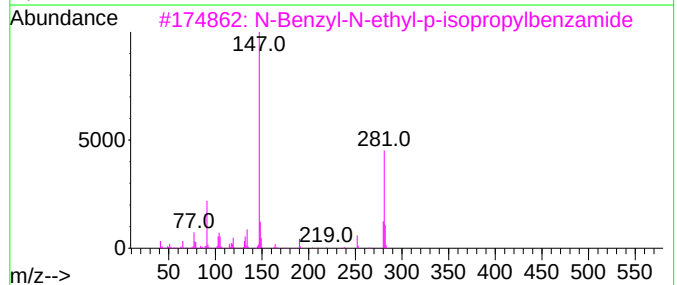
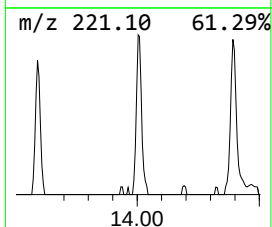
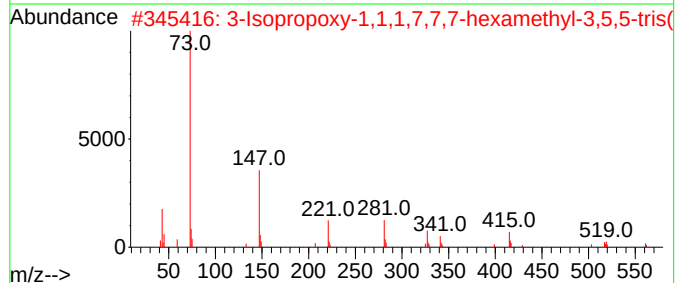
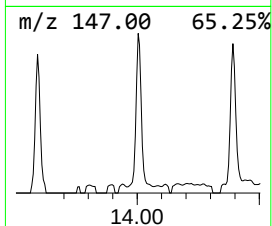
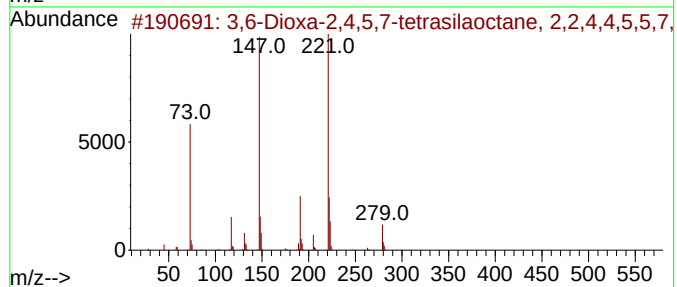
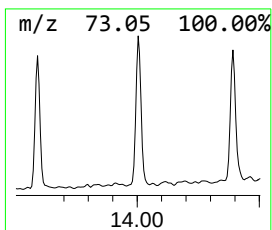
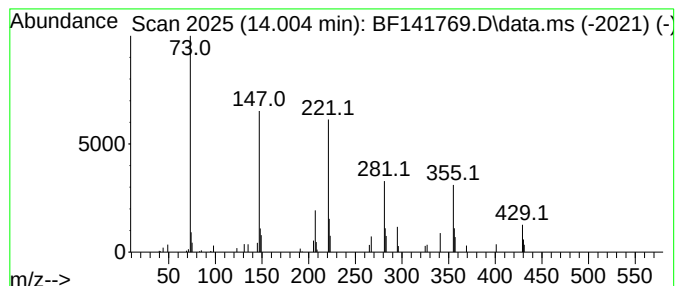
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.004 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	2.13 ng	44363	Chrysene-d12	13.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	35	
2	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	32	
3	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27	
4	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27	
5	Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	25	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141769.D
Acq On : 25 Feb 2025 17:34
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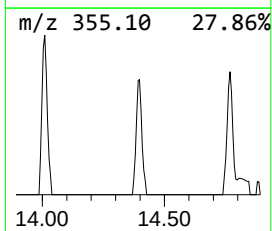
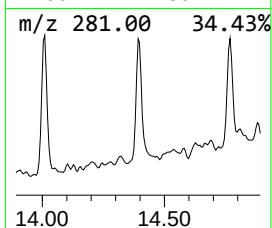
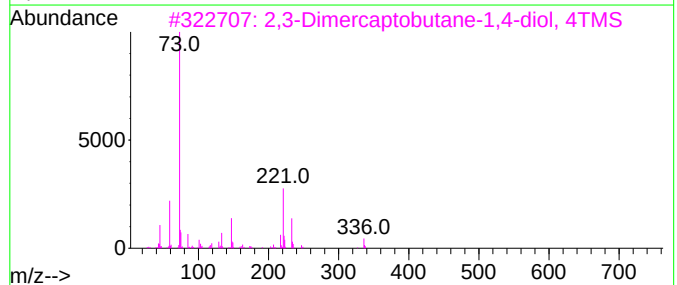
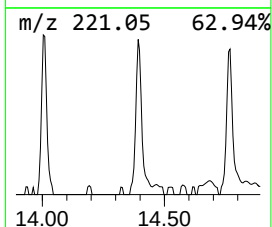
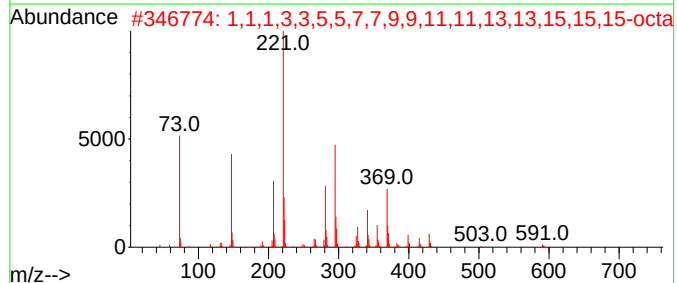
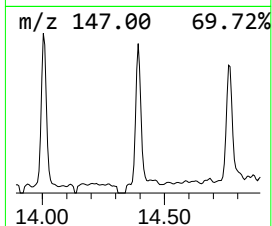
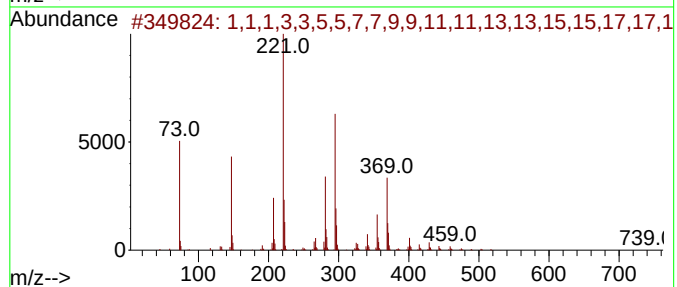
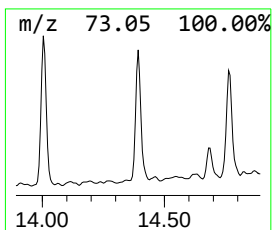
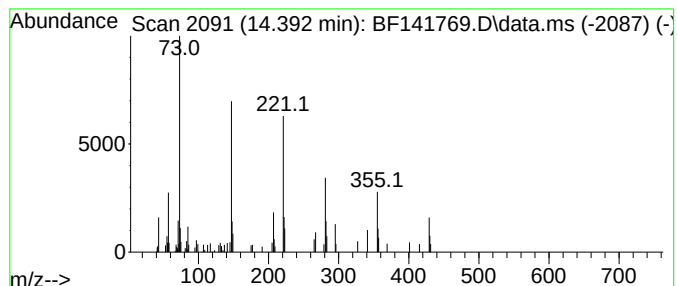
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.392 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	2.61 ng	54244	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	42		
2	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	40		
3	2,3-Dimercaptobutane-1,4-diol, 4TMS	442	C16H42O2S2Si4	959295-06-8	38		
4	3,6-Dioxo-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32		
5	Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	32		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
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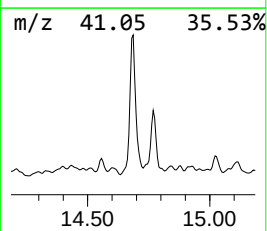
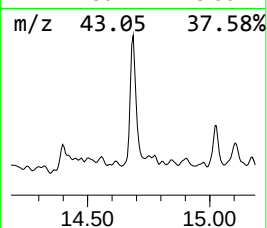
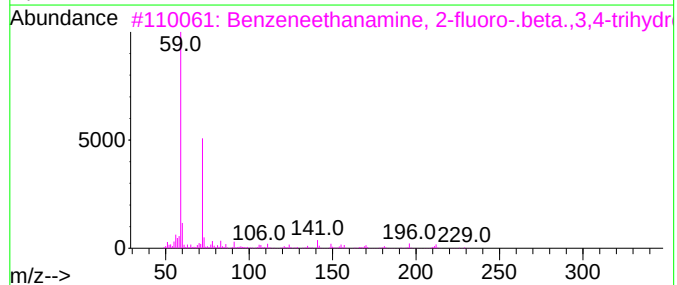
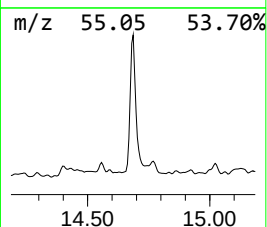
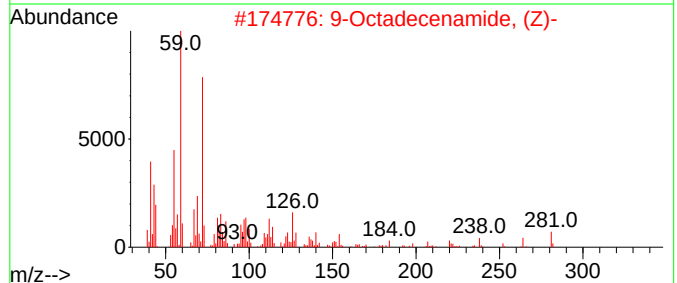
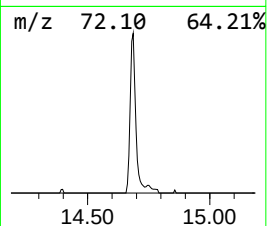
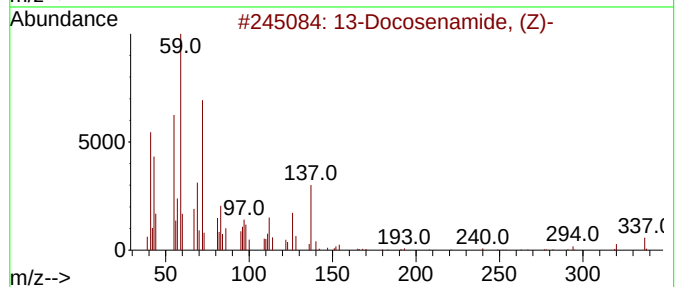
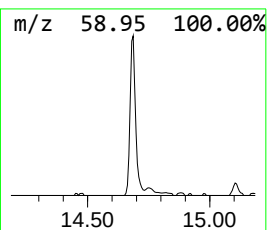
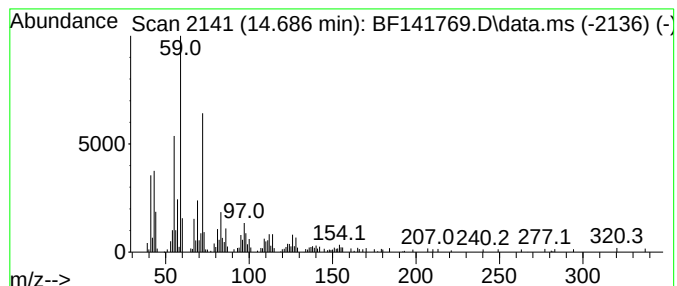
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.686	6.51 ng	153482	Perylene-d12	15.380

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
5		Palmitoleamide	253	C16H31NO	106010-22-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141769.D
Acq On : 25 Feb 2025 17:34
Operator : RC/JU
Sample : Q1415-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-163-SB01

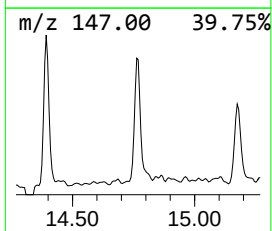
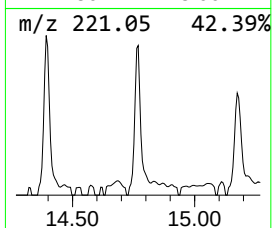
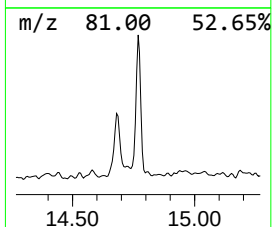
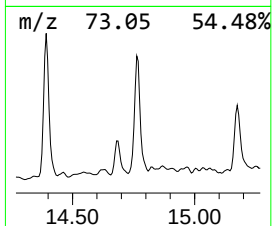
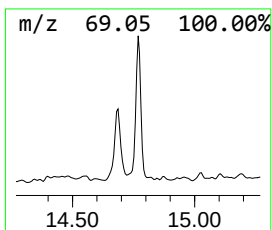
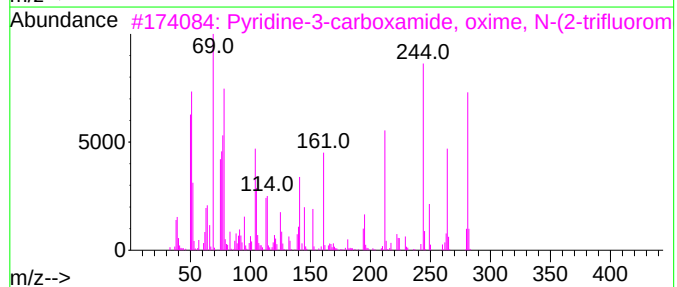
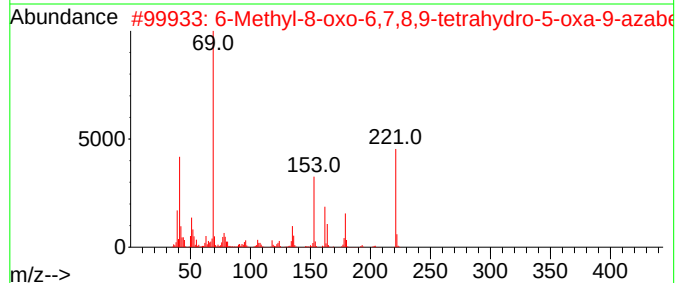
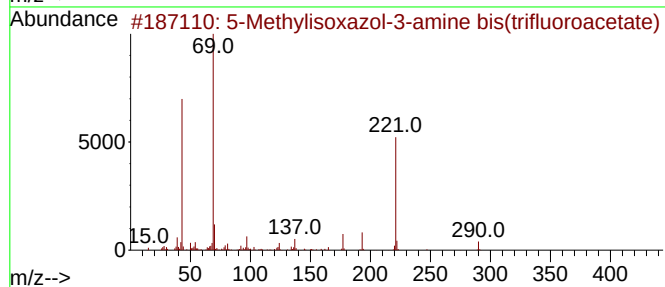
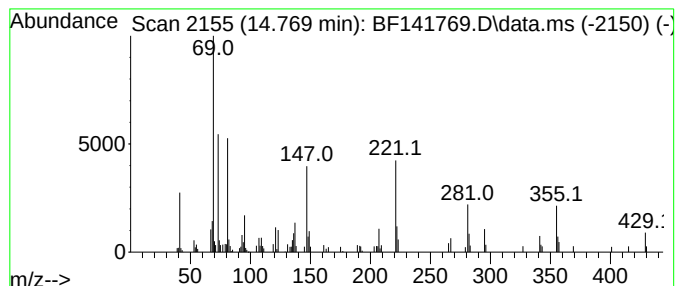
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown14.769 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.769	3.30 ng	77876	Perylene-d12	15.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Methylisoxazol-3-amine bis(tri...	290	C8H4F6N2O3	1000373-35-6	37
2			6-Methyl-8-oxo-6,7,8,9-tetrahydr...	221	C11H11N04	134076-69-0	37
3			Pyridine-3-carboxamide, oxime, N...	281	C13H10F3N3O	288246-53-7	27
4			1-Bromo-11-iodoundecane	360	C11H22BrI	139123-69-6	27
5			2-Amino-4,6-dihydroxypyrimidine,...	415	C10H2F9N3O5	1000375-76-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022525\
Data File : BF141769.D
Acq On : 25 Feb 2025 17:34
Operator : RC/JU
Sample : Q1415-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-163-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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
unknown2.293	2.293	2.8	ng	53463	1	6.781	386466	20.0
2-Butenoic acid...	2.540	37.5	ng	724892	1	6.781	386466	20.0
unknown3.216	3.216	6.2	ng	118915	1	6.781	386466	20.0
Diethyl carbonate	4.175	27.3	ng	527025	1	6.781	386466	20.0
Hexanedioic aci...	8.787	7.5	ng	179623	2	8.063	481091	20.0
Benzophenone	10.528	4.5	ng	107009	3	9.816	477546	20.0
unknown10.851	10.851	2.6	ng	56107	4	11.298	438056	20.0
n-Hexadecanoic ...	11.828	5.7	ng	125203	4	11.298	438056	20.0
Heptadecyl hept...	13.780	6.6	ng	137269	5	13.939	415698	20.0
unknown14.004	14.004	2.1	ng	44363	5	13.939	415698	20.0
unknown14.392	14.392	2.6	ng	54244	5	13.939	415698	20.0
13-Docosenamide...	14.686	6.5	ng	153482	6	15.380	471646	20.0
unknown14.769	14.769	3.3	ng	77876	6	15.380	471646	20.0