

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
 Data File : BF142446.D
 Acq On : 19 May 2025 12:39
 Operator : RC/JU
 Sample : Q2032-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-11

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF050525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.434	206	211	229	rBV	68358	157276	5.60%	0.708%
2	5.122	492	498	504	rVB	166957	239926	8.54%	1.079%
3	5.516	559	565	571	rBV	1558707	2084689	74.23%	9.379%
4	6.151	669	673	679	rBV2	20553	38417	1.37%	0.173%
5	6.451	719	724	730	rVV6	10693	29709	1.06%	0.134%
6	6.522	730	736	748	rVB	1609050	2204865	78.51%	9.920%
7	6.728	767	771	780	rVB	36895	60023	2.14%	0.270%
8	6.904	792	801	806	rVB	658053	874973	31.16%	3.936%
9	7.175	843	847	851	rVB	22555	29785	1.06%	0.134%
10	7.298	864	868	871	rBV3	20995	28287	1.01%	0.127%
11	7.463	885	896	905	rBV	1025480	1467140	52.24%	6.601%
12	7.539	905	909	914	rVV5	21474	35088	1.25%	0.158%
13	7.598	914	919	924	rBV2	20358	36092	1.29%	0.162%
14	7.710	935	938	945	rVB2	39377	55706	1.98%	0.251%
15	7.786	946	951	955	rBV5	20171	42126	1.50%	0.190%
16	8.133	1005	1010	1013	rBV4	13985	29409	1.05%	0.132%
17	8.186	1013	1019	1024	rVV	824703	1137080	40.49%	5.116%
18	8.239	1024	1028	1031	rVV2	47984	72890	2.60%	0.328%
19	8.269	1031	1033	1041	rVB8	21841	36011	1.28%	0.162%
20	8.492	1063	1071	1080	rVB	123846	222408	7.92%	1.001%
21	8.598	1086	1089	1094	rBV	23861	33693	1.20%	0.152%
22	9.257	1195	1201	1206	rBV	2251343	2808341	100.00%	12.635%
23	9.939	1311	1317	1322	rBV	1007295	1252696	44.61%	5.636%
24	10.028	1326	1332	1342	rVV	121323	191860	6.83%	0.863%
25	10.239	1362	1368	1381	rBV	34550	105207	3.75%	0.473%
26	10.357	1382	1388	1404	rVB3	17321	48607	1.73%	0.219%
27	10.651	1432	1438	1445	rBV	70143	94899	3.38%	0.427%
28	10.727	1445	1451	1464	rBV	1432823	1869865	66.58%	8.413%
29	11.427	1564	1570	1577	rBV	1033742	1341647	47.77%	6.036%
30	11.492	1577	1581	1586	rVB3	25369	38258	1.36%	0.172%
31	11.951	1651	1659	1671	rBV2	338667	582409	20.74%	2.620%
32	12.039	1671	1674	1682	rVB4	13408	29156	1.04%	0.131%
33	12.639	1772	1776	1785	rBV	48931	72834	2.59%	0.328%
34	12.733	1787	1792	1806	rVV	124330	221833	7.90%	0.998%
35	12.868	1810	1815	1818	rVV	43355	64742	2.31%	0.291%
36	12.904	1818	1821	1831	rVB2	26761	39082	1.39%	0.176%

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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-BF050525.M
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37	13.010	1834	1839	1845	rVV	2060000	2725200	97.04%	12.261%
38	13.904	1987	1991	2003	rBV	72513	136243	4.85%	0.613%
39	14.063	2013	2018	2036	rVB	629037	895423	31.88%	4.029%
40	15.557	2266	2272	2284	rVB	496776	793293	28.25%	3.569%

Sum of corrected areas: 22227188

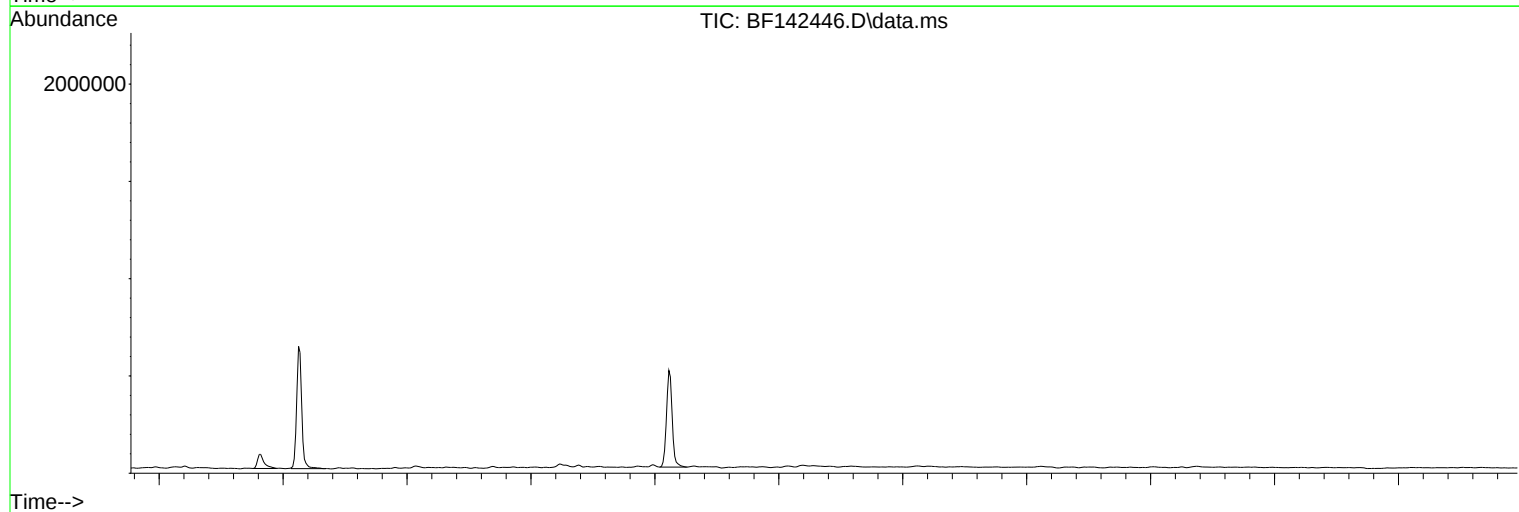
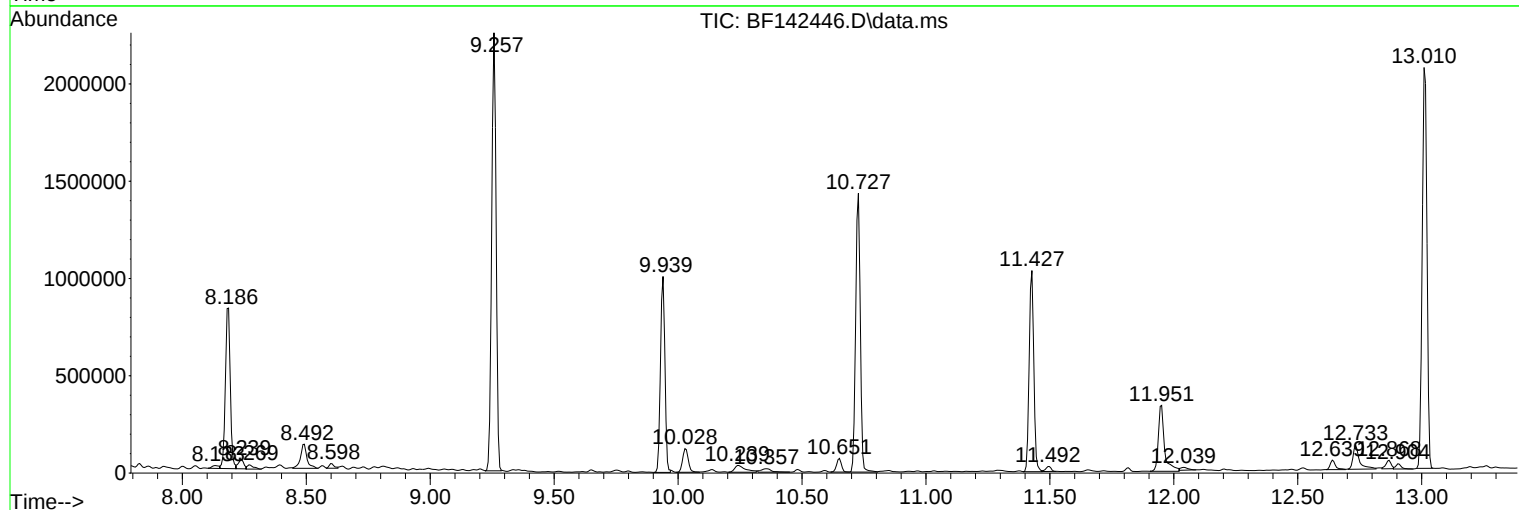
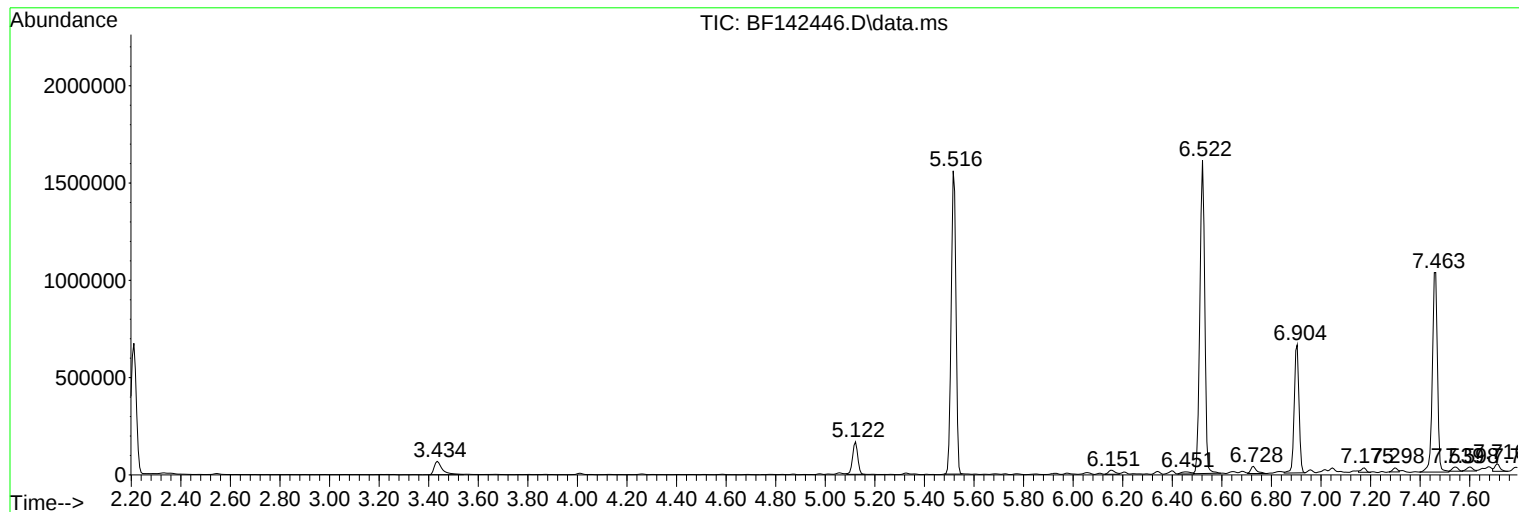
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Operator : RC/JU
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

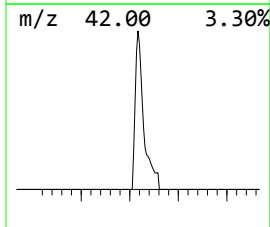
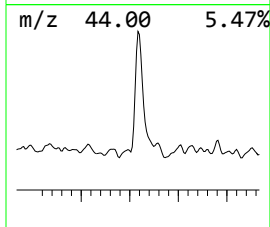
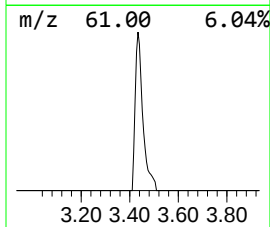
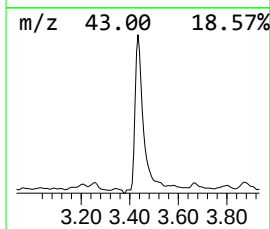
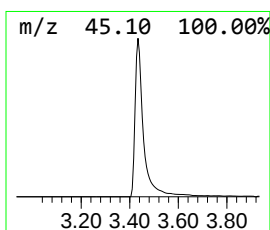
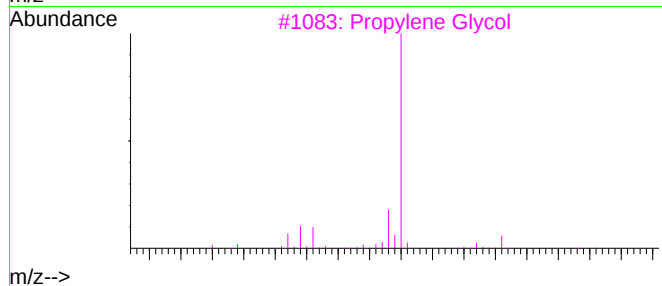
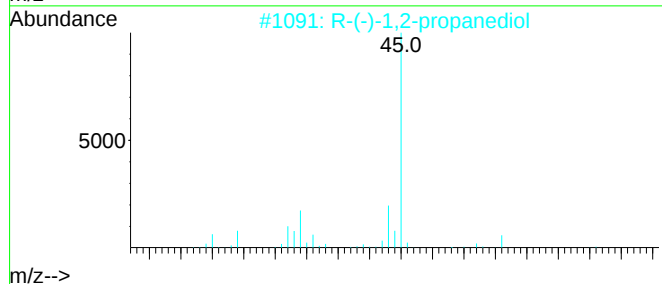
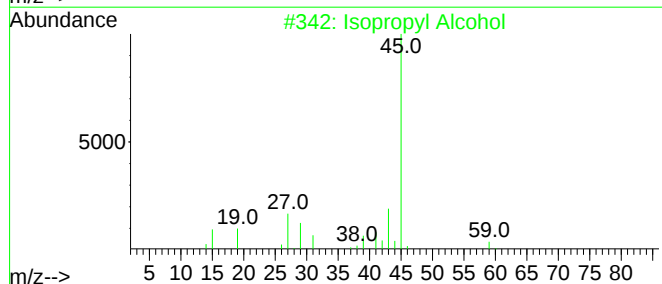
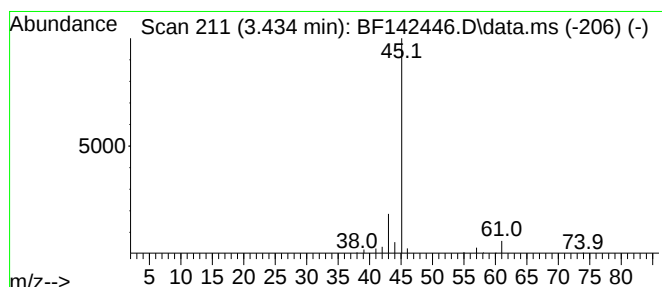
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.434	3.59 ng	157276	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	43
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9



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TP-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

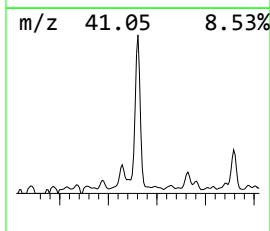
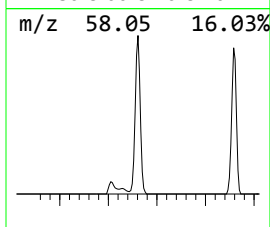
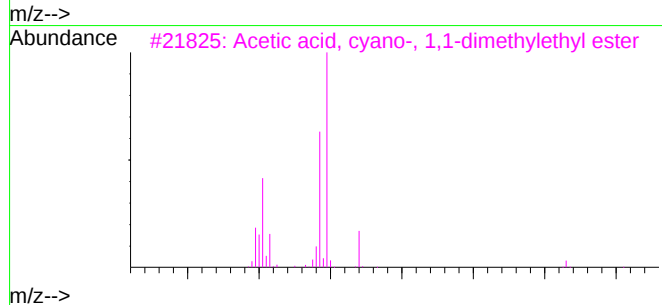
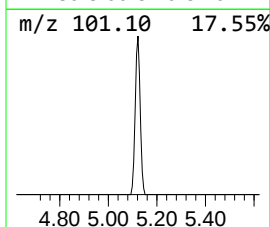
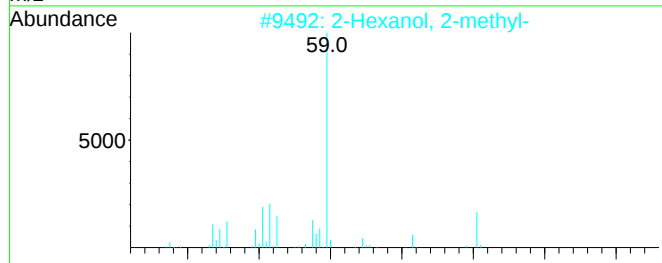
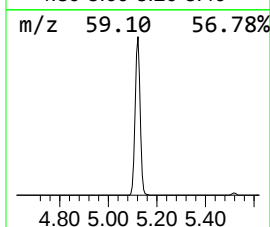
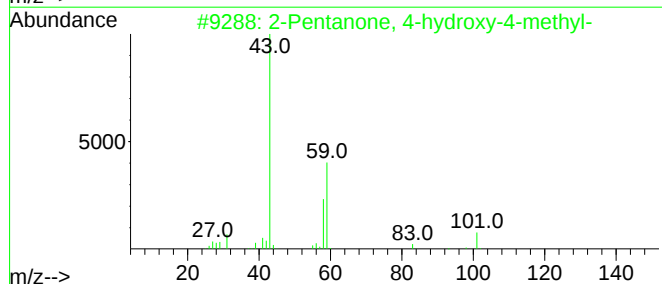
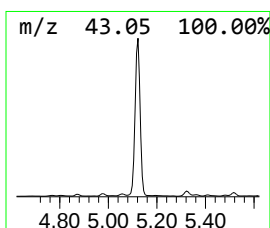
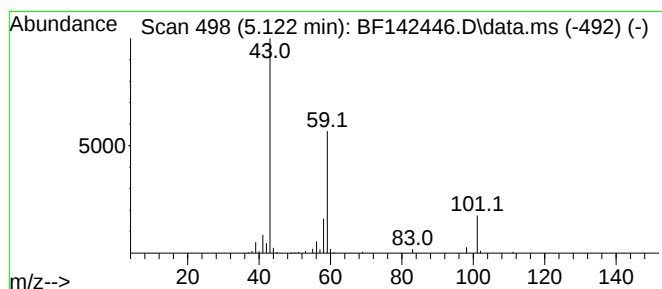
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	5.48 ng	239926	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
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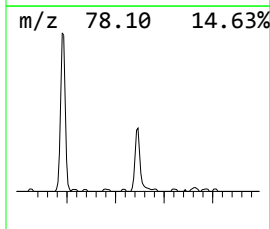
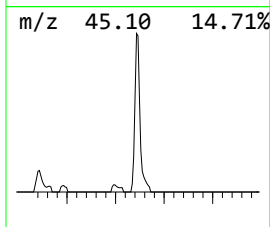
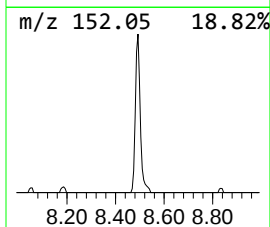
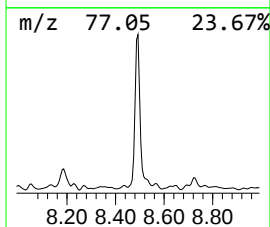
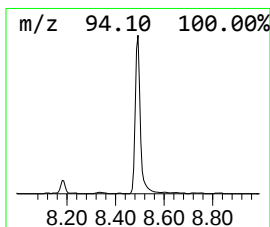
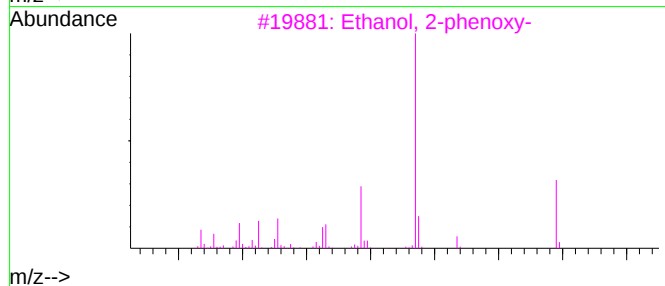
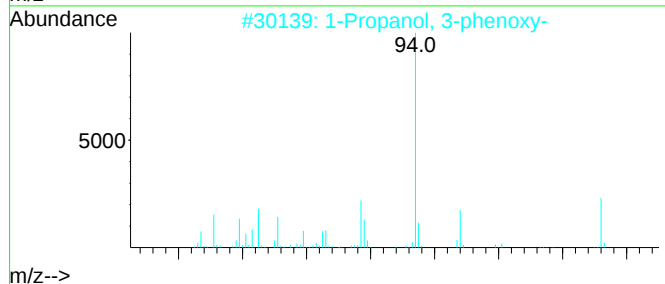
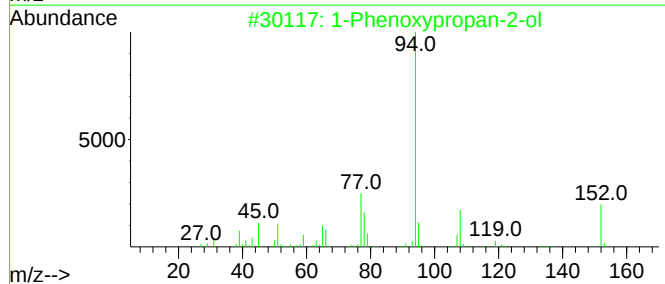
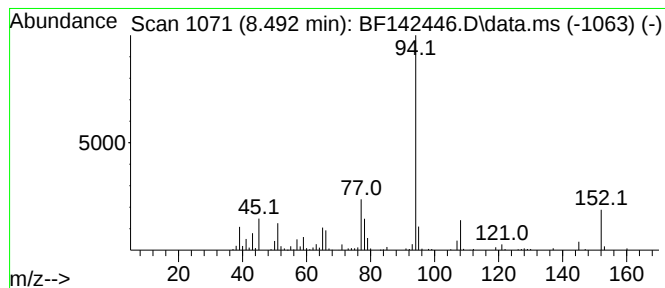
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.492	3.91 ng	222408	Naphthalene-d8	8.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	93
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5	tert-Butyl phenyl carbonate	194	C11H14O3	006627-89-0	53



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
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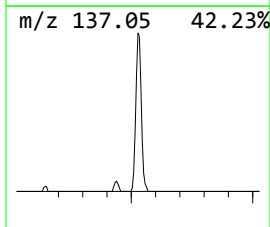
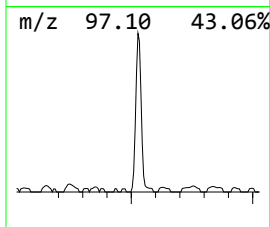
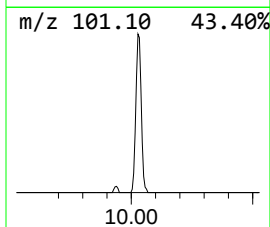
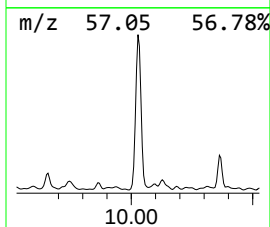
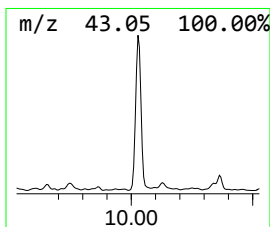
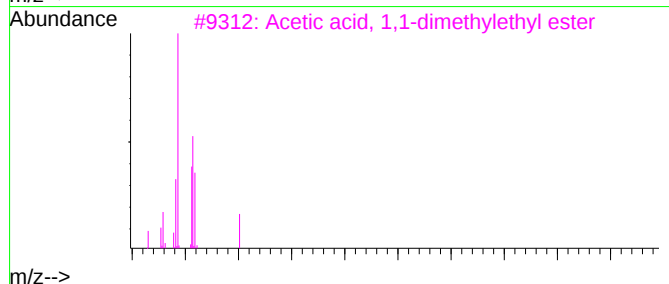
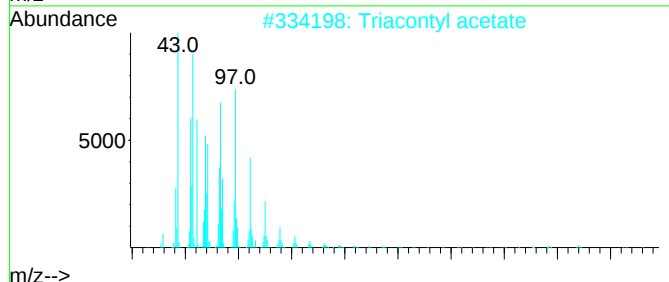
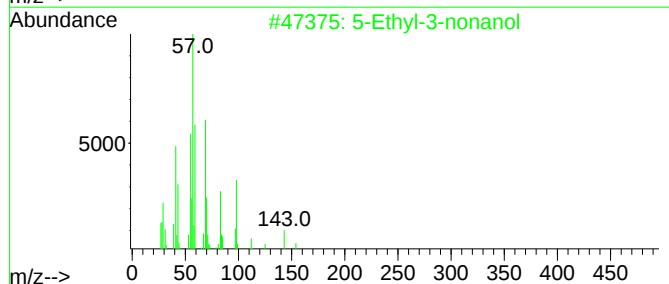
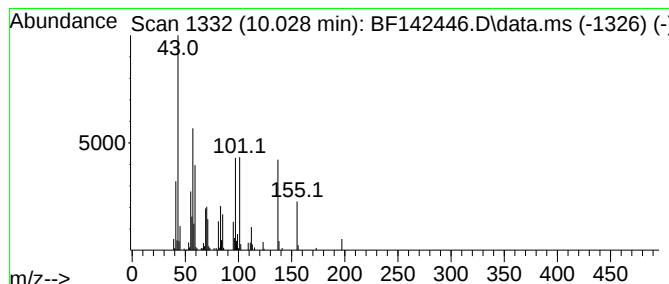
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown10.028 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.028	3.06 ng	191860	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyl-3-nonanol	172	C11H24O	019780-71-3	12
2	Triacetyl acetate	480	C32H64O2	041755-58-2	10
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
4	Pentanoic acid, 4,4-dimethyl-3-o...	158	C8H14O3	055107-14-7	10
5	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10



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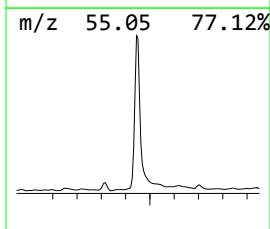
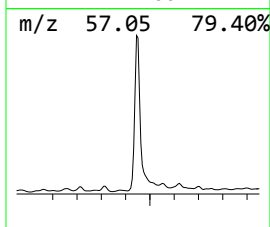
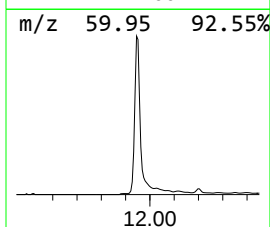
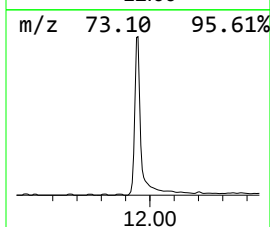
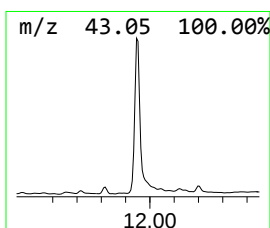
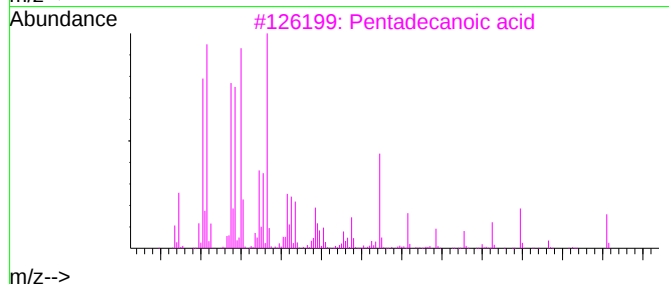
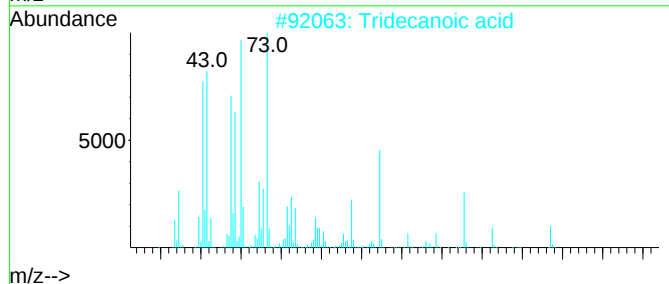
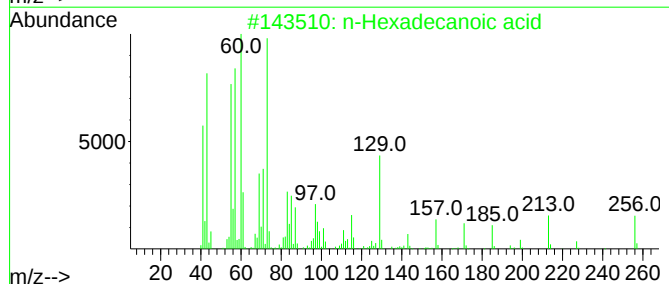
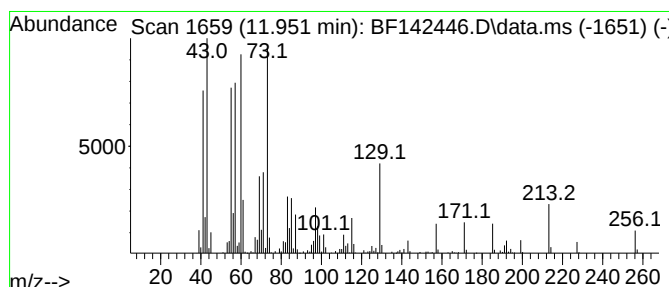
Instrument :
BNA_F
ClientSampleId :
TP-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
11.951	8.68 ng	582409	Phenanthrene-d10		11.427	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	64
5	n-Decanoic acid		172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142446.D
Acq On : 19 May 2025 12:39
Operator : RC/JU
Sample : Q2032-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

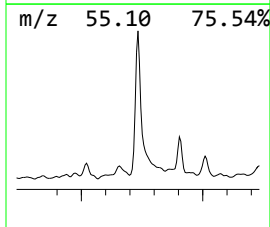
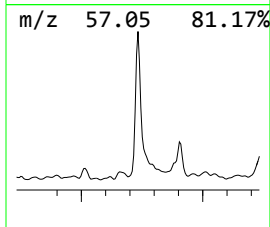
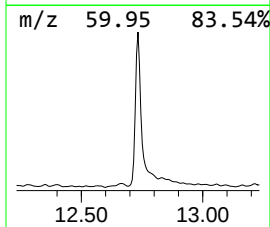
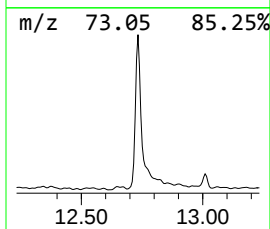
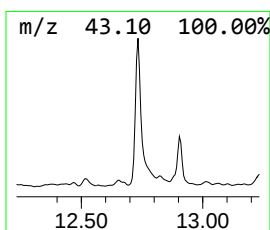
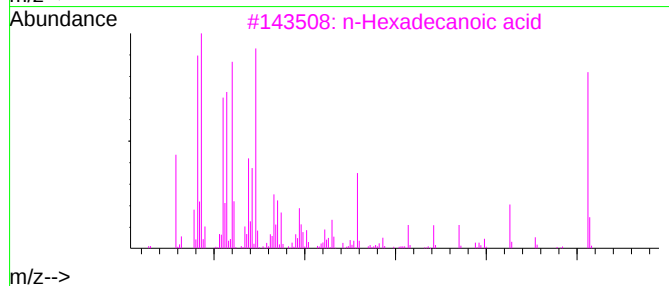
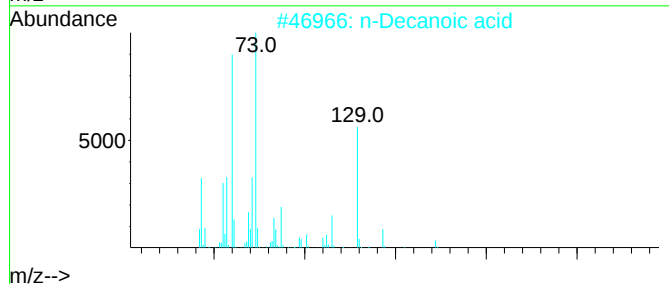
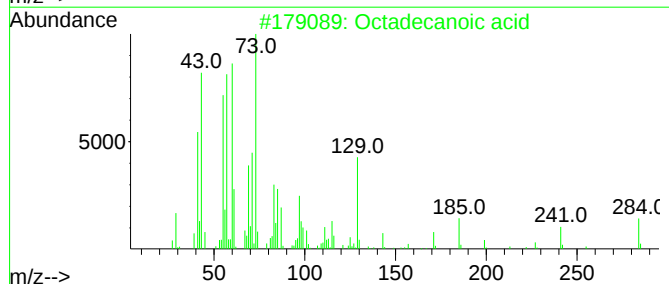
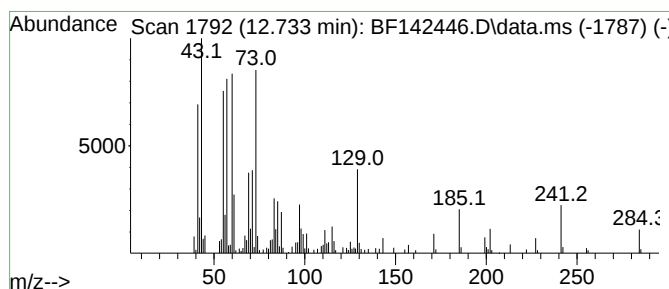
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
12.733	3.31 ng	221833	Phenanthrene-d10		11.427	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	n-Decanoic acid		172	C10H20O2	000334-48-5	93
3	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	93
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	83
5	Pentadecanoic acid		242	C15H30O2	001002-84-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142446.D
Acq On : 19 May 2025 12:39
Operator : RC/JU
Sample : Q2032-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11

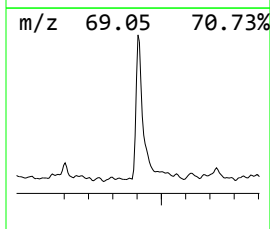
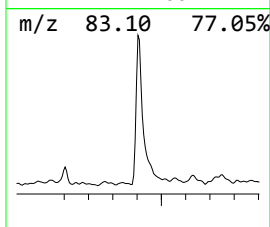
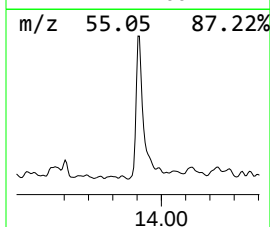
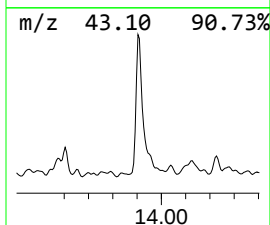
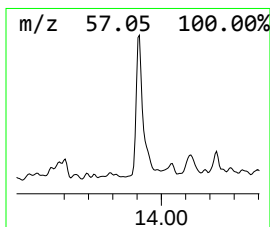
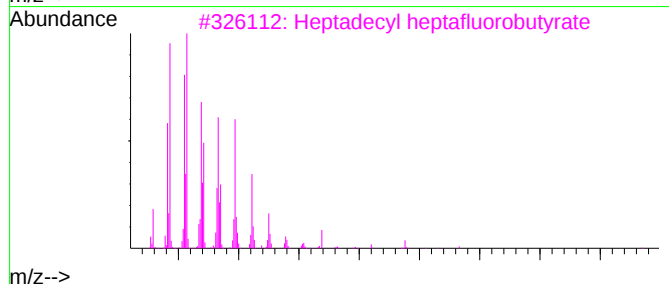
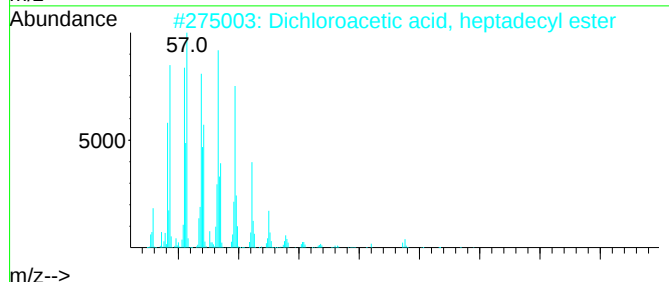
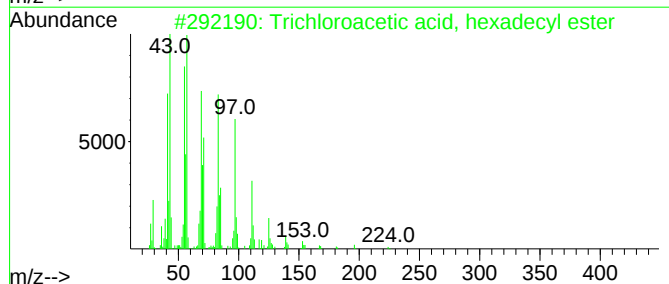
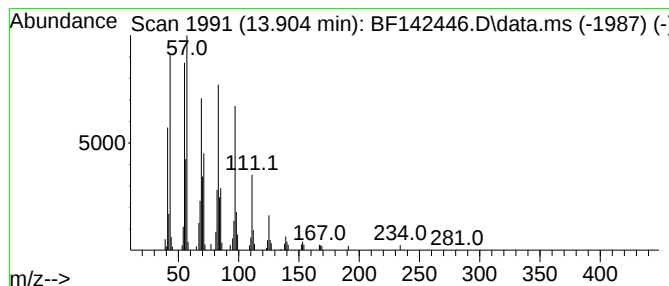
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.904	3.04 ng	136243	Chrysene-d12		14.063	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	95
2	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	95
3	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94
4	1-Hexacosene		364	C26H52	018835-33-1	94
5	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142446.D
Acq On : 19 May 2025 12:39
Operator : RC/JU
Sample : Q2032-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.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
Isopropyl Alcohol	3.434	3.6	ng	157276	1	6.904	874973	20.0
2-Pentanone, 4-...	5.122	5.5	ng	239926	1	6.904	874973	20.0
1-Phenoxypropan...	8.492	3.9	ng	222408	2	8.186	1137080	20.0
unknown10.028	10.028	3.1	ng	191860	3	9.939	1252700	20.0
n-Hexadecanoic ...	11.951	8.7	ng	582409	4	11.427	1341650	20.0
Octadecanoic acid	12.733	3.3	ng	221833	4	11.427	1341650	20.0
Trichloroacetic...	13.904	3.0	ng	136243	5	14.063	895423	20.0