

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
 Data File : BF139096.D
 Acq On : 21 Aug 2024 12:21
 Operator : RC/JU
 Sample : P3663-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 916-J-SD-0-0.5-081624

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-BF082024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139096.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	11	18	30	rVB	1053860	1591932	99.30%	11.185%
2	2.305	31	36	42	rBV	10617	16544	1.03%	0.116%
3	3.393	216	221	232	rBV	28223	63700	3.97%	0.448%
4	3.993	317	323	332	rVB	20484	31750	1.98%	0.223%
5	5.110	504	513	519	rVB	69529	102793	6.41%	0.722%
6	5.510	575	581	586	rBV	1191060	1538824	95.99%	10.812%
7	6.510	745	751	756	rBV	1193800	1603149	100.00%	11.264%
8	6.716	781	786	797	rVB	23442	30149	1.88%	0.212%
9	6.893	811	816	821	rBV	440724	555004	34.62%	3.899%
10	7.051	835	843	847	rBV	55184	67473	4.21%	0.474%
11	7.451	905	911	916	rBV	763064	979644	61.11%	6.883%
12	8.175	1029	1034	1039	rBV	574736	720217	44.93%	5.060%
13	8.487	1082	1087	1093	rBV	35973	45085	2.81%	0.317%
14	9.251	1211	1217	1222	rBV	1316544	1599729	99.79%	11.240%
15	9.934	1327	1333	1338	rBV	643991	819553	51.12%	5.758%
16	10.028	1344	1349	1356	rBV	33349	51651	3.22%	0.363%
17	10.716	1461	1466	1471	rBV	851194	1039943	64.87%	7.307%
18	11.416	1580	1585	1593	rVB	633181	787082	49.10%	5.530%
19	11.528	1600	1604	1608	rBV	16439	20930	1.31%	0.147%
20	11.851	1655	1659	1667	rVB3	28518	35388	2.21%	0.249%
21	11.945	1667	1675	1679	rBV	59679	92922	5.80%	0.653%
22	12.628	1786	1791	1797	rBV	17963	22988	1.43%	0.162%
23	12.728	1804	1808	1818	rBV2	22913	33335	2.08%	0.234%
24	12.857	1822	1830	1834	rBV	16112	23276	1.45%	0.164%
25	13.004	1849	1855	1860	rVB	887354	1095685	68.35%	7.698%
26	13.904	2003	2008	2016	rBV	52885	88164	5.50%	0.619%
27	14.051	2028	2033	2042	rBV	313726	412676	25.74%	2.899%
28	14.539	2111	2116	2124	rBV	40204	69518	4.34%	0.488%
29	15.098	2206	2211	2221	rBV	9513	20738	1.29%	0.146%
30	15.198	2223	2228	2239	rBV3	20399	46460	2.90%	0.326%
31	15.533	2279	2285	2291	rBV	313550	477316	29.77%	3.354%
32	15.798	2325	2330	2336	rVB5	10745	19288	1.20%	0.136%
33	16.039	2366	2371	2375	rBV2	10364	17364	1.08%	0.122%
34	16.086	2375	2379	2387	rVB3	12807	25642	1.60%	0.180%
35	17.727	2653	2658	2667	rVB8	8936	19170	1.20%	0.135%
36	17.980	2694	2701	2709	rBV7	18011	42193	2.63%	0.296%

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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-BF082024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.462	2778	2783	2795	rBV10	9636	25781	1.61%	0.181%
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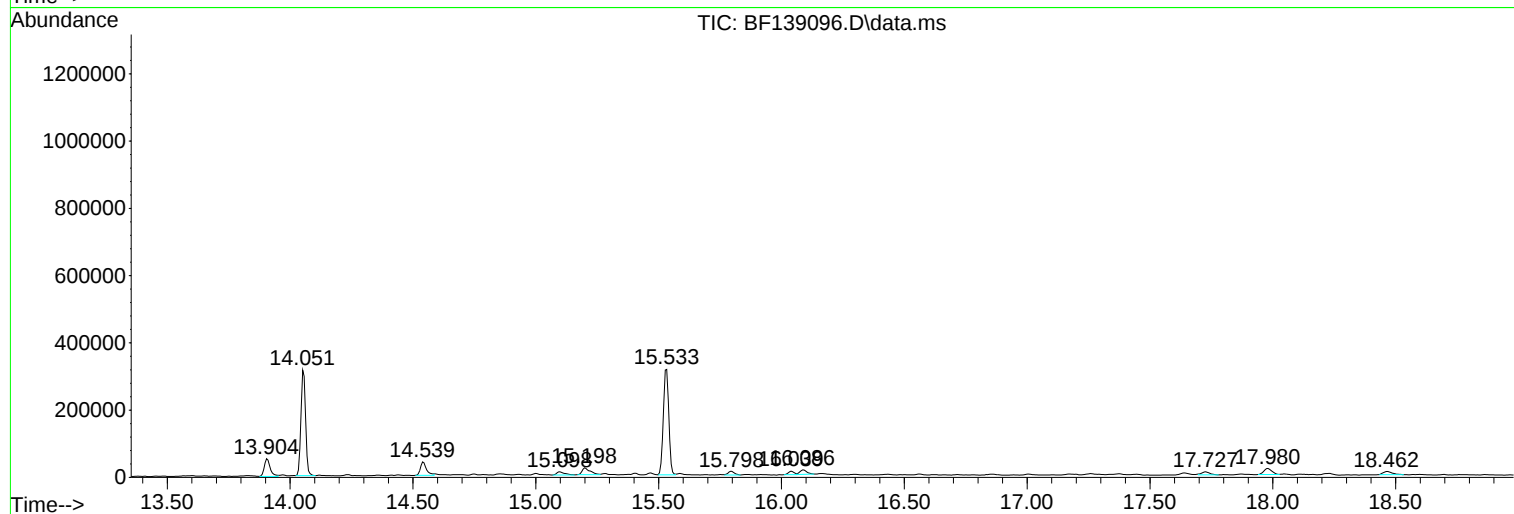
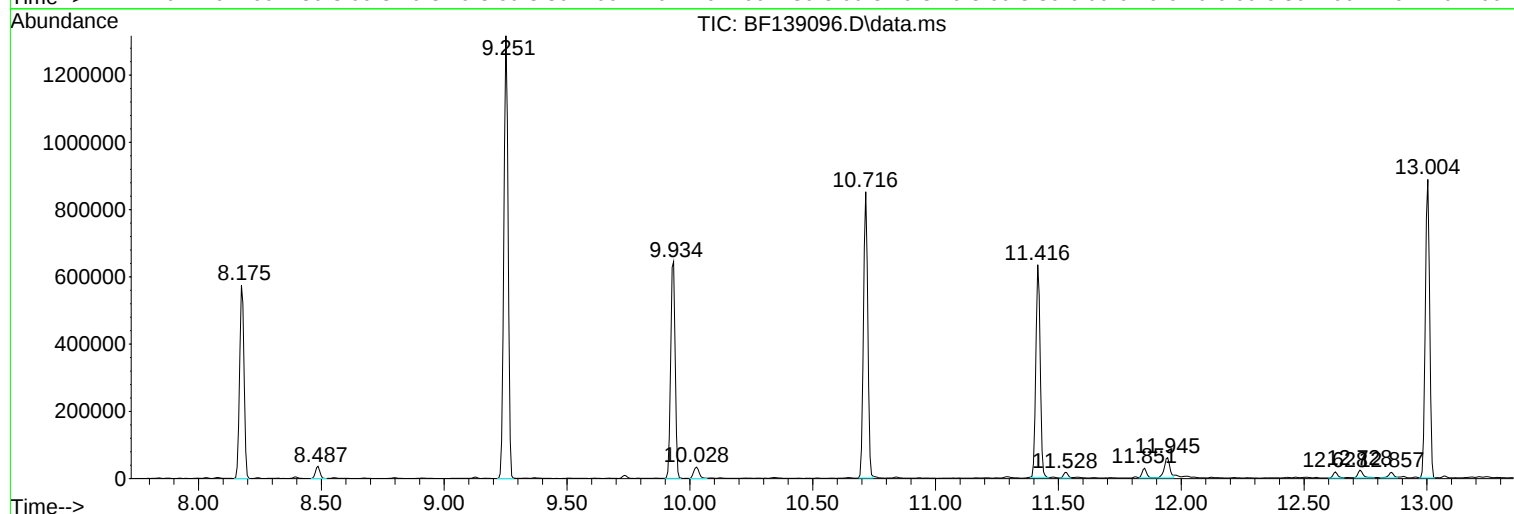
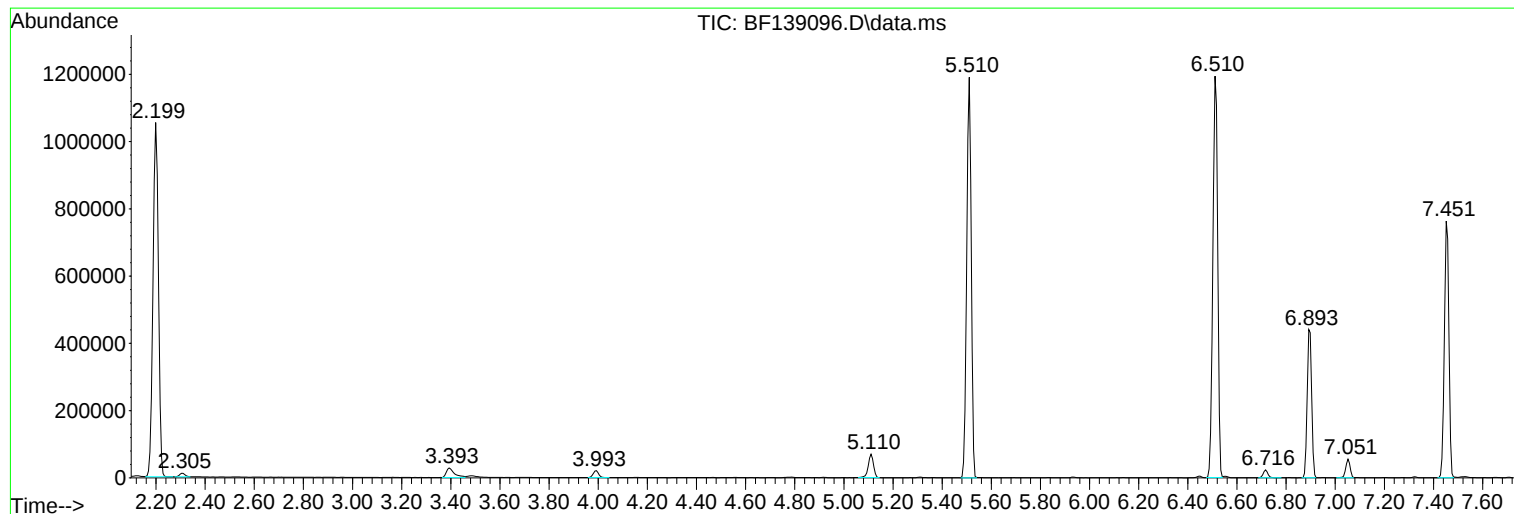
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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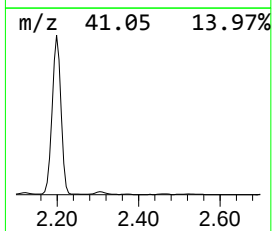
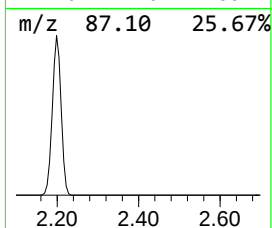
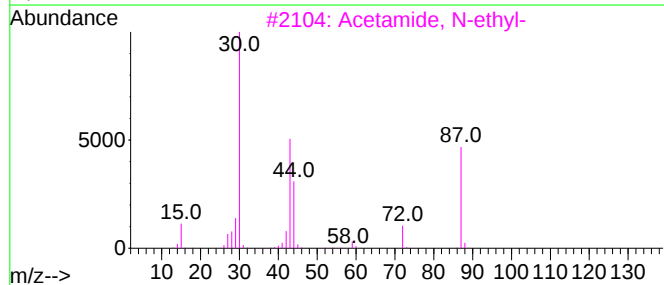
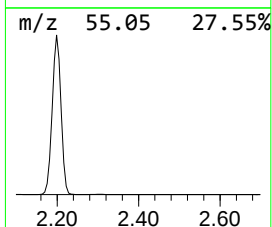
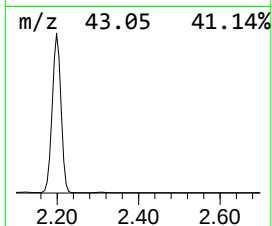
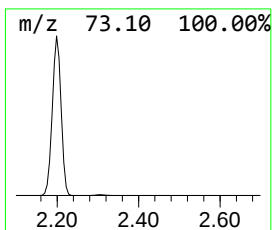
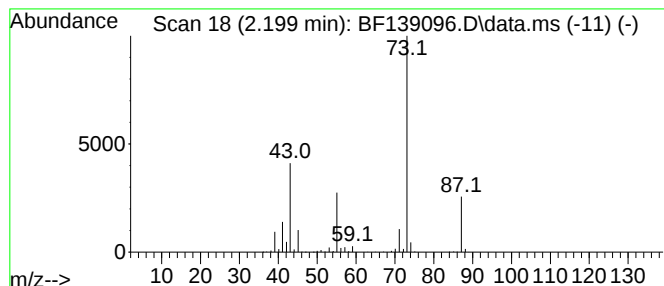
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	57.37 ng	1591930	1,4-Dichlorobenzene-d4	6.898

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	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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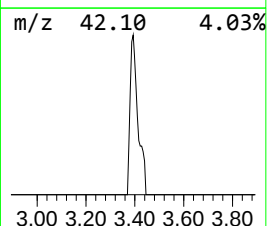
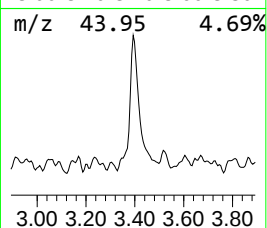
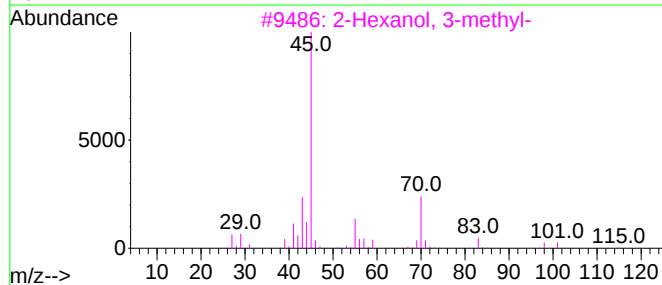
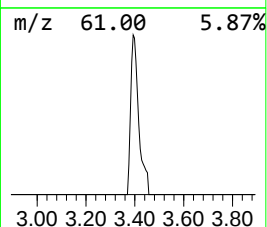
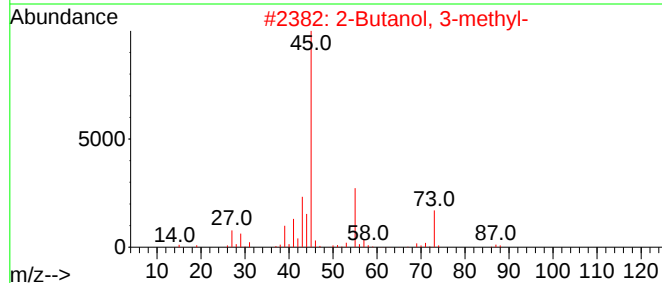
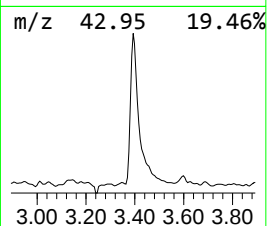
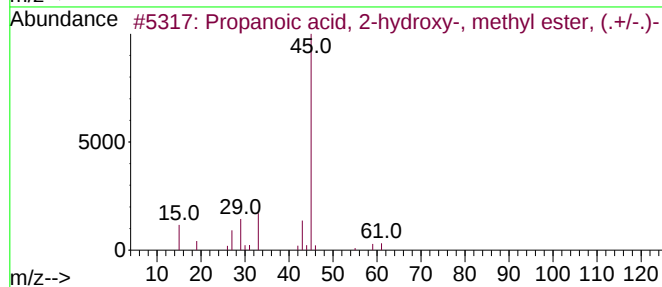
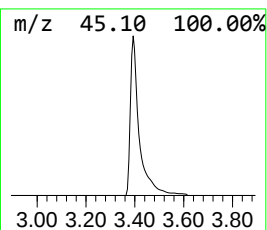
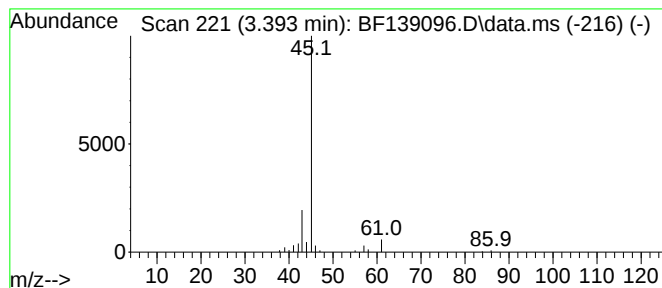
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.393 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	2.30 ng	63700	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
2			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
3			2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	9
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5			Propylene Glycol	76	C3H8O2	000057-55-6	9



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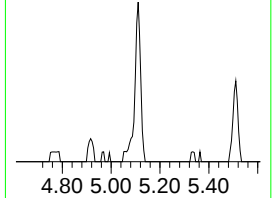
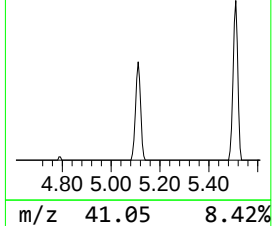
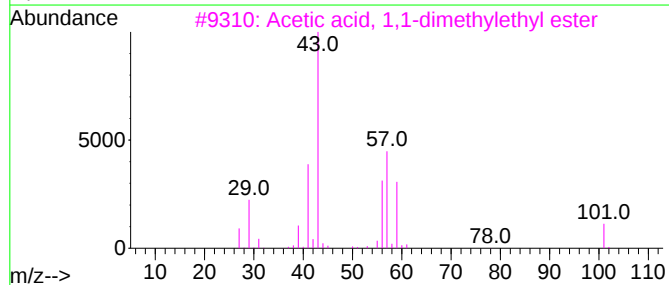
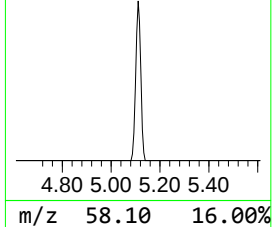
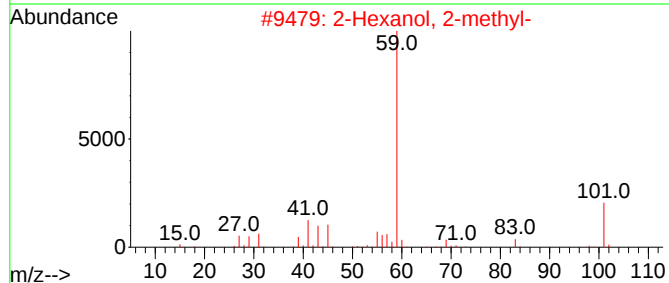
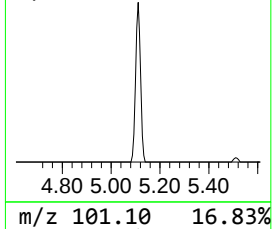
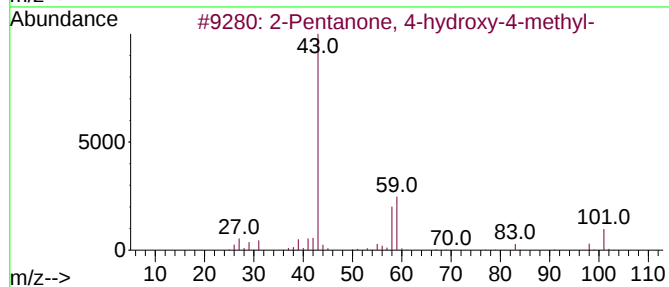
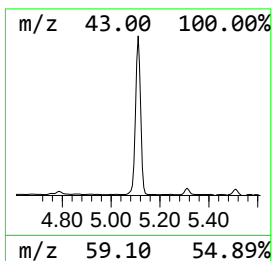
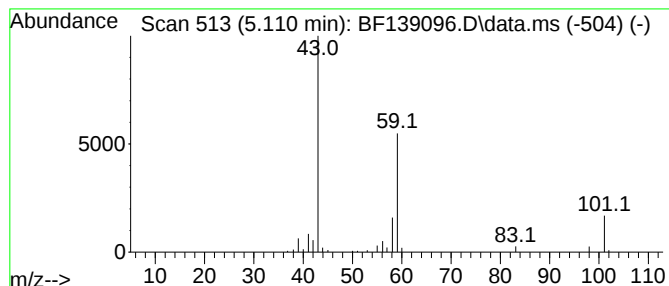
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	3.70 ng	102793	1,4-Dichlorobenzene-d4	6.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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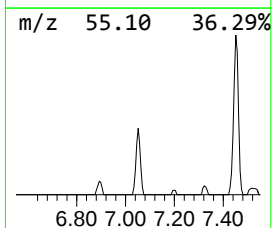
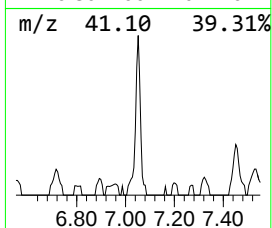
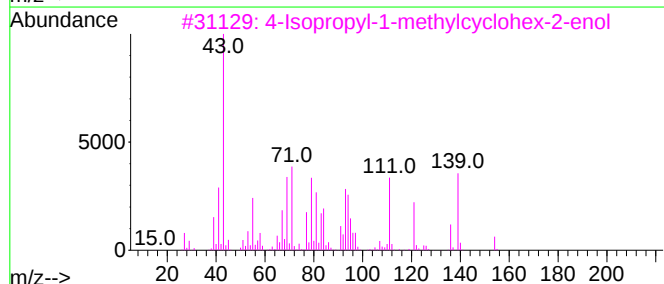
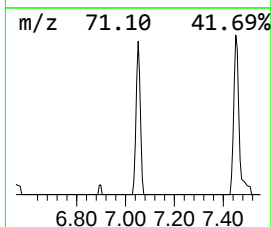
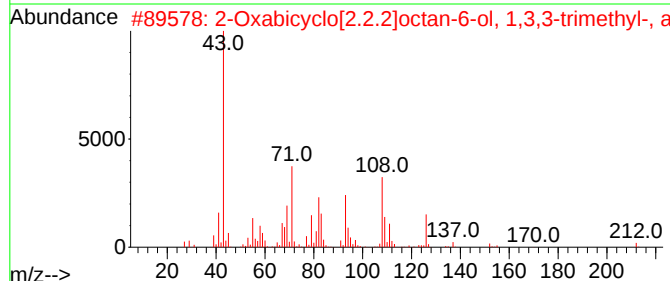
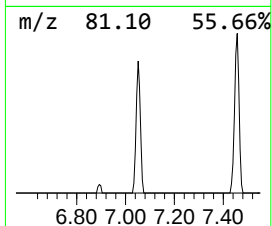
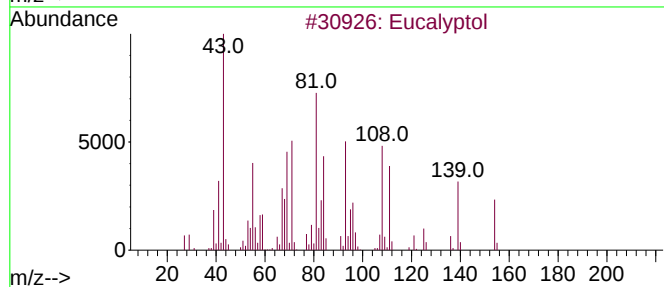
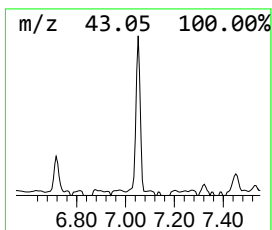
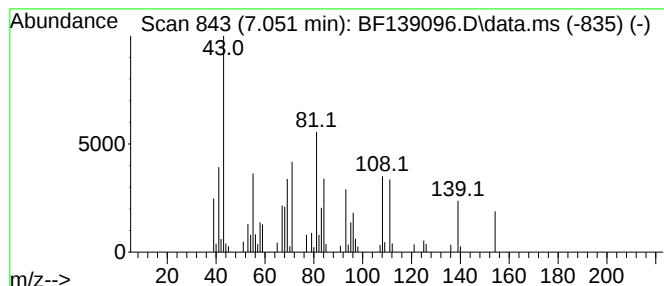
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.051	2.43 ng	67473	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	93
2			2-Oxabicyclo[2.2.2]octan-6-ol, 1...	212	C12H20O3	057709-95-2	47
3			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	40
4			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	35
5			7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	32



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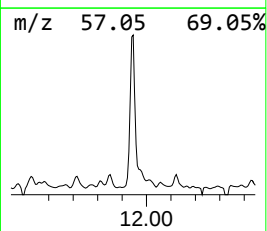
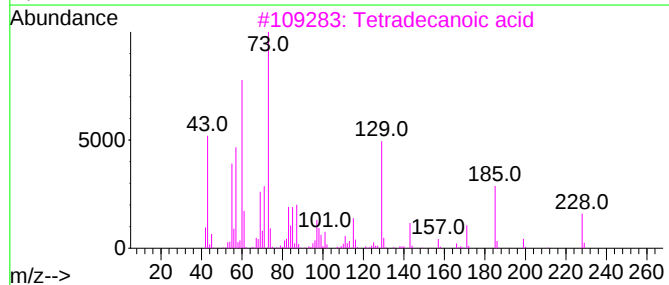
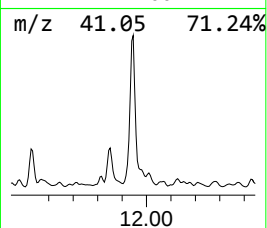
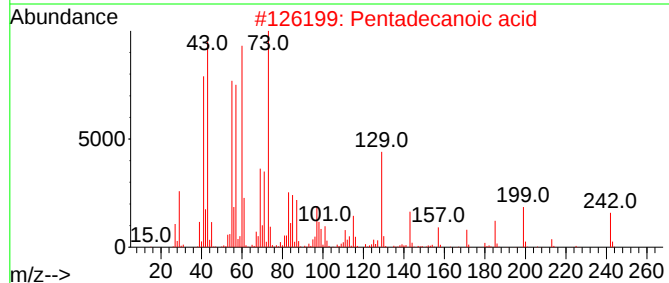
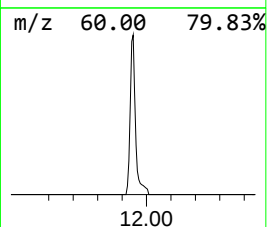
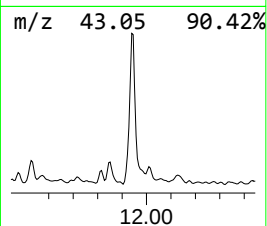
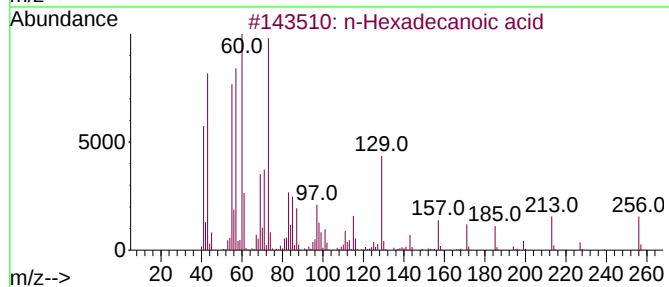
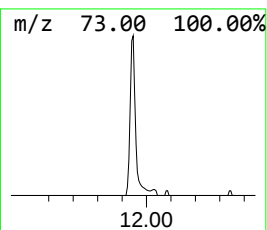
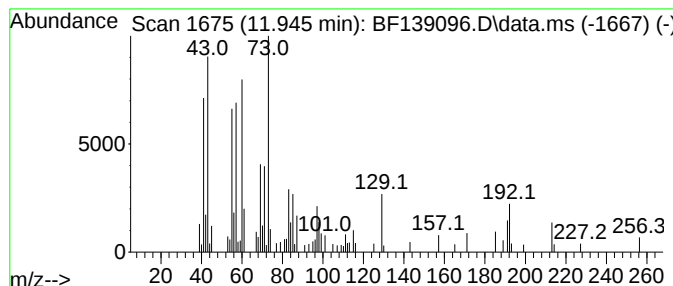
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.36 ng	92922	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5			Hexadecyl nonyl ether	368	C25H52O	1000406-37-7	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139096.D
Acq On : 21 Aug 2024 12:21
Operator : RC/JU
Sample : P3663-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0-0.5-081624

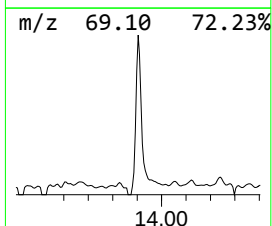
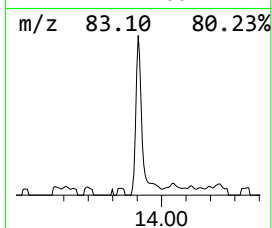
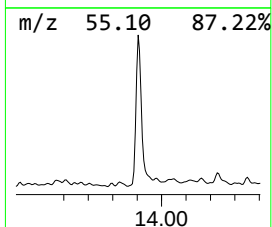
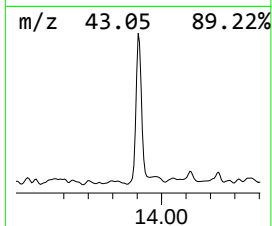
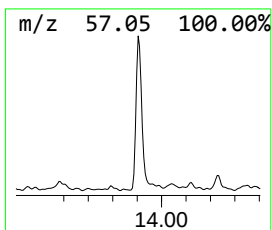
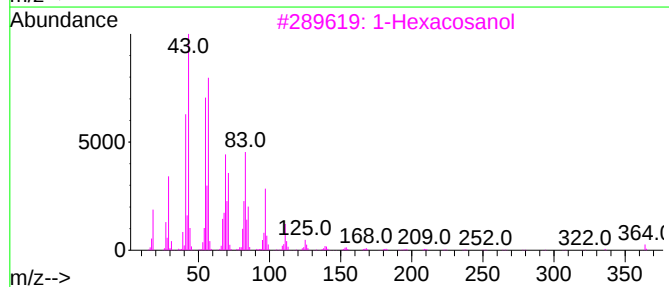
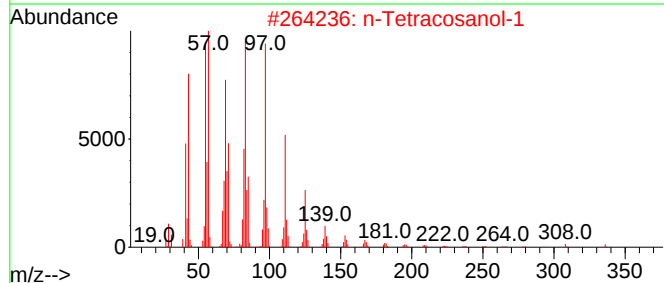
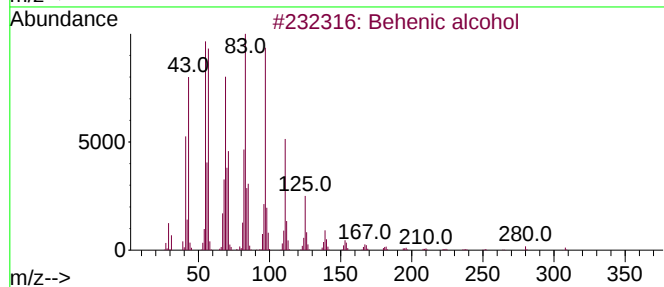
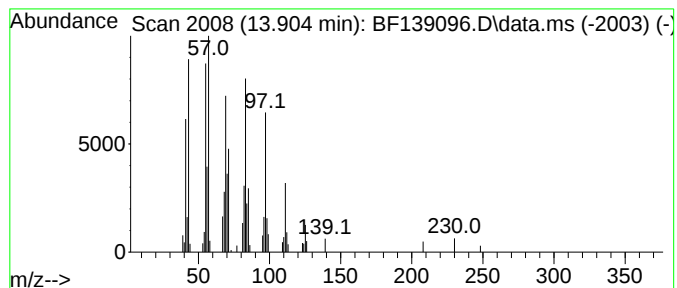
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	4.27 ng	88164	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			1-Hexacosanol	382	C26H54O	000506-52-5	91
4			1-Heptacosanol	396	C27H56O	002004-39-9	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139096.D
Acq On : 21 Aug 2024 12:21
Operator : RC/JU
Sample : P3663-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0-0.5-081624

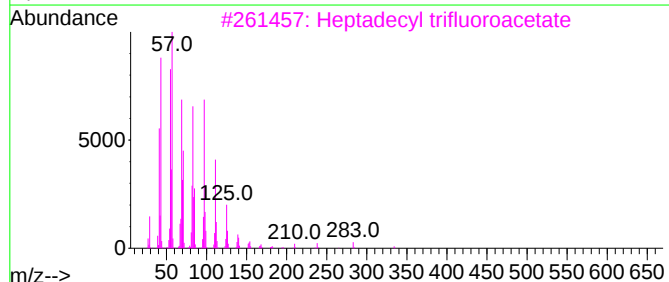
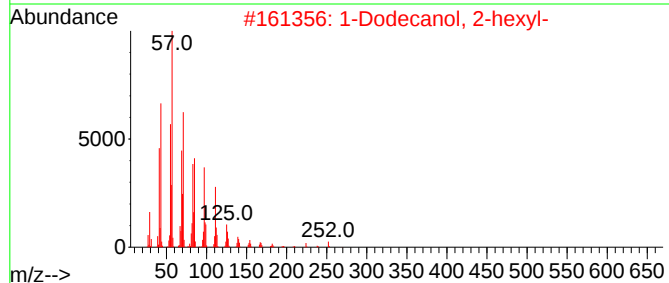
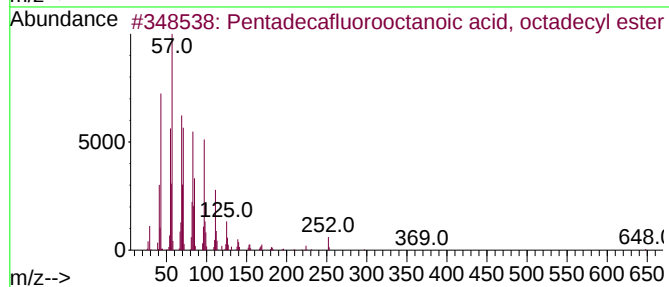
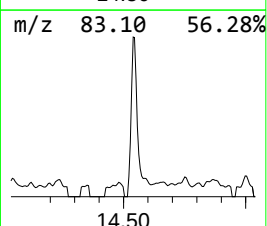
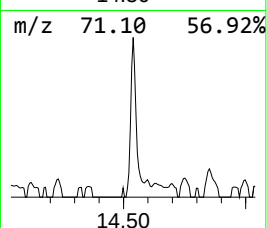
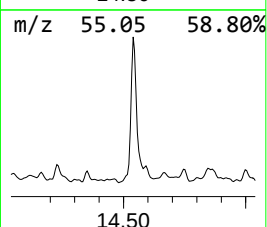
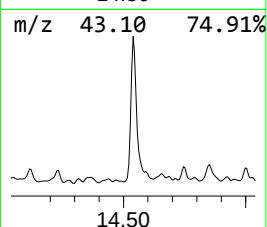
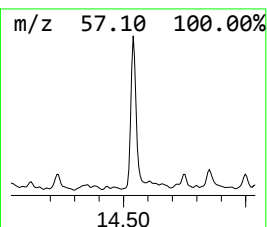
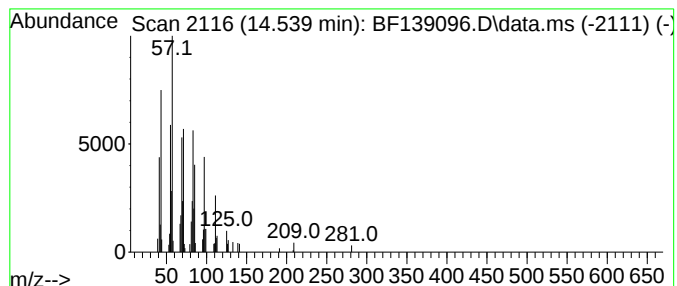
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	3.37 ng	69518	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
2			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	83
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	76
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	76
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
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Sample : P3663-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0-0.5-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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
Butane, 2-metho...	2.199	57.4	ng	1591930	1	6.898	555004	20.0
unknown3.393	3.393	2.3	ng	63700	1	6.898	555004	20.0
2-Pentanone, 4-...	5.110	3.7	ng	102793	1	6.898	555004	20.0
Eucalyptol	7.051	2.4	ng	67473	1	6.898	555004	20.0
n-Hexadecanoic ...	11.945	2.4	ng	92922	4	11.416	787082	20.0
Behenic alcohol	13.904	4.3	ng	88164	5	14.051	412676	20.0
Pentadecafluoro...	14.539	3.4	ng	69518	5	14.051	412676	20.0