

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
 Data File : BF138445.D
 Acq On : 03 Jul 2024 14:44
 Operator : CG\JU
 Sample : P3141-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-129-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-BF062824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138445.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	10	17	22	rBV	2783956	3489981	91.14%	11.754%
2	2.293	30	35	40	rBV	41744	50314	1.31%	0.169%
3	3.410	221	225	238	rBV	60328	130275	3.40%	0.439%
4	5.093	508	511	524	rVB	385116	485469	12.68%	1.635%
5	5.499	576	580	584	rBV	3853561	3738297	97.62%	12.590%
6	6.504	746	751	754	rBV	3489207	3499900	91.40%	11.787%
7	6.698	781	784	787	rBV2	48364	46353	1.21%	0.156%
8	6.869	809	813	817	rVB	1159070	934558	24.41%	3.148%
9	6.928	817	823	830	rBV2	66589	62073	1.62%	0.209%
10	7.434	903	909	912	rBV	2340956	2231933	58.28%	7.517%
11	7.681	943	951	956	rVB	113483	95937	2.51%	0.323%
12	8.151	1023	1031	1034	rBV	1444167	1213360	31.69%	4.087%
13	8.457	1074	1083	1087	rBV	132225	148381	3.87%	0.500%
14	8.740	1127	1131	1135	rVB	109048	98846	2.58%	0.333%
15	9.228	1208	1214	1217	rBV	4390953	3829370	100.00%	12.897%
16	9.304	1223	1227	1230	rBV	126576	106864	2.79%	0.360%
17	9.834	1313	1317	1319	rBV	52850	42801	1.12%	0.144%
18	9.904	1325	1329	1332	rBV	1716463	1333062	34.81%	4.490%
19	9.998	1340	1345	1350	rBV2	126981	167103	4.36%	0.563%
20	10.692	1459	1463	1466	rBV	2288717	1933817	50.50%	6.513%
21	11.386	1578	1581	1584	rBV	1200640	1099435	28.71%	3.703%
22	11.910	1664	1670	1683	rBV2	155965	219023	5.72%	0.738%
23	12.598	1784	1787	1790	rBV	56406	50846	1.33%	0.171%
24	12.786	1815	1819	1822	rBV	179676	157476	4.11%	0.530%
25	12.827	1823	1826	1831	rVB	42616	46533	1.22%	0.157%
26	12.975	1847	1851	1853	rBV	2839760	2399500	62.66%	8.081%
27	12.992	1853	1854	1861	rVB	211442	137260	3.58%	0.462%
28	13.510	1939	1942	1945	rBV	171565	140010	3.66%	0.472%
29	13.874	2000	2004	2019	rBV2	130022	238154	6.22%	0.802%
30	14.027	2023	2030	2033	rBV	845242	814520	21.27%	2.743%
31	14.492	2106	2109	2112	rBV	44623	44422	1.16%	0.150%
32	15.492	2274	2279	2289	rBV	547159	705851	18.43%	2.377%

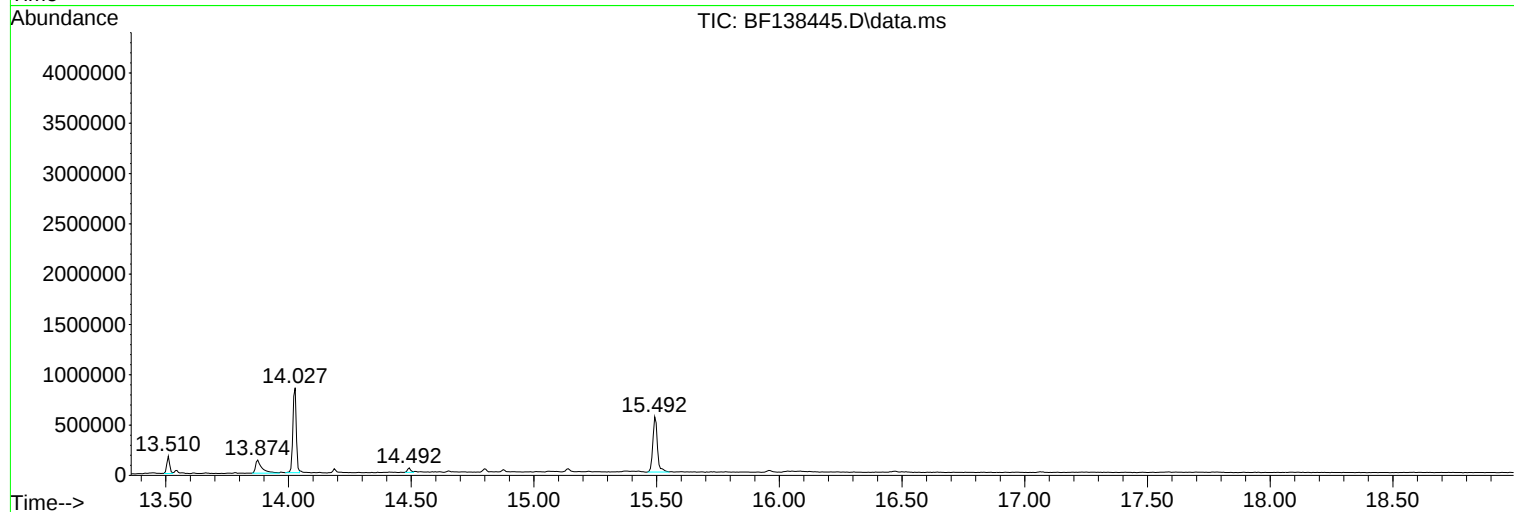
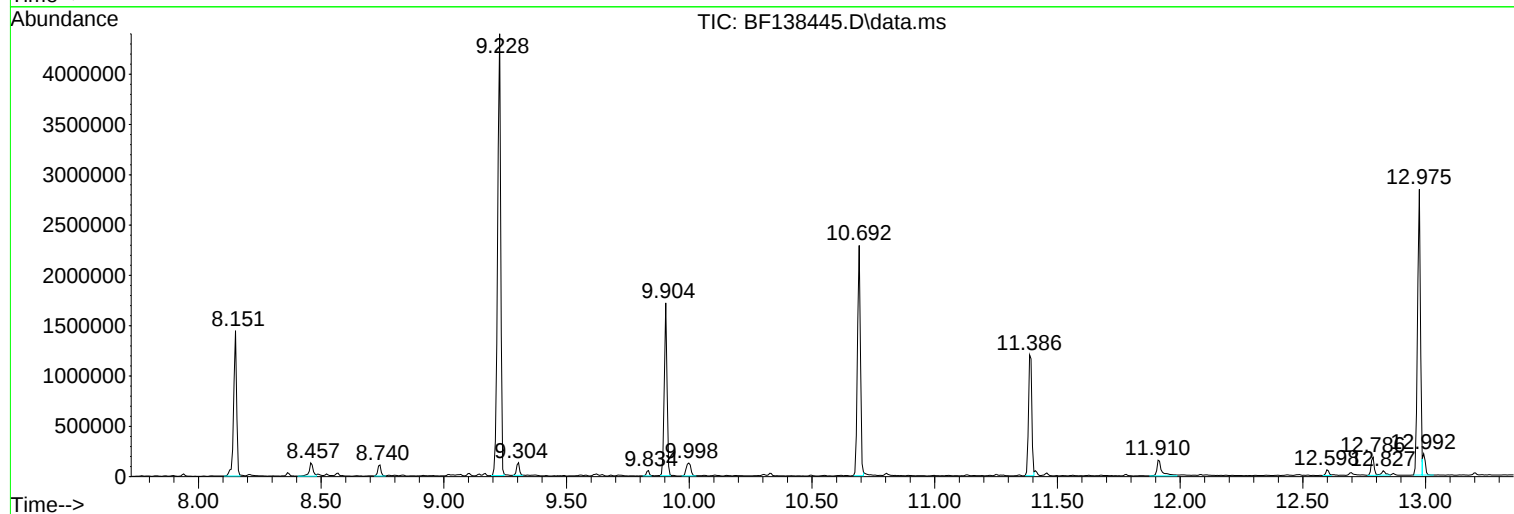
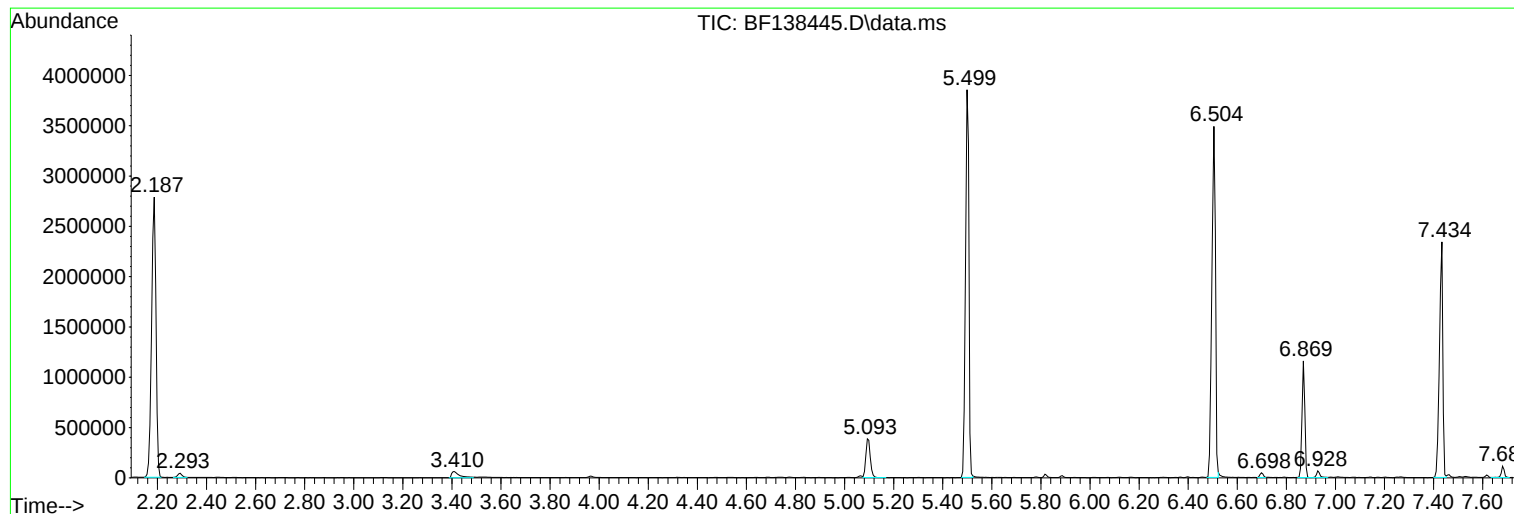
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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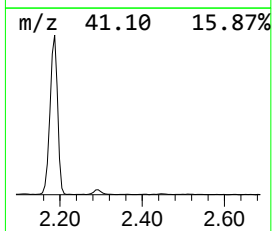
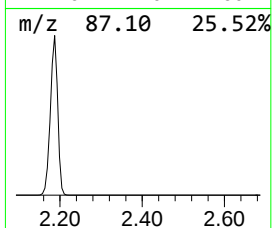
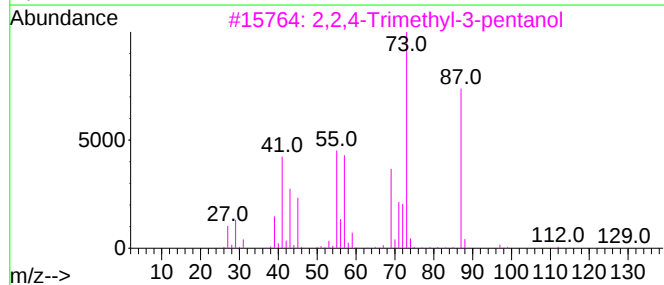
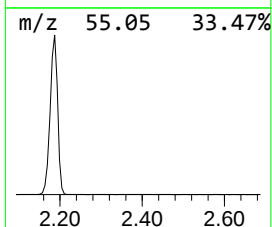
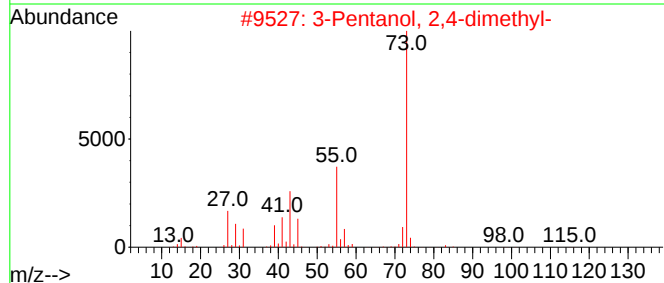
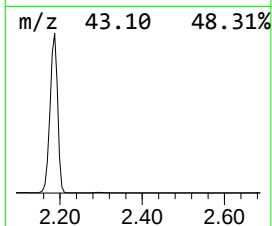
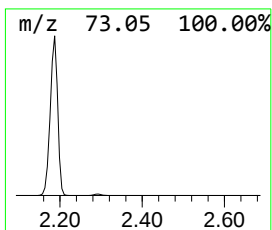
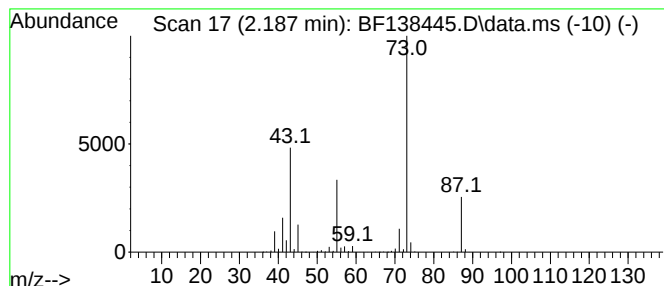
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	74.69 ng	3489980	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37



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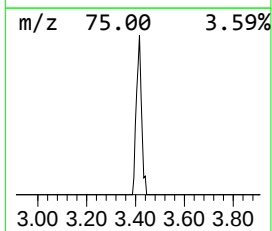
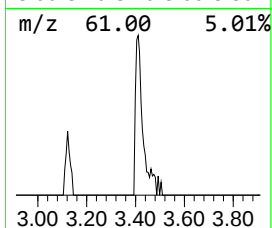
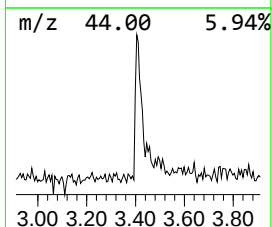
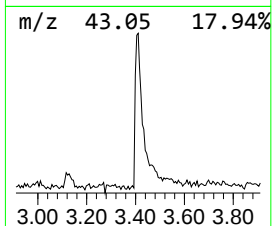
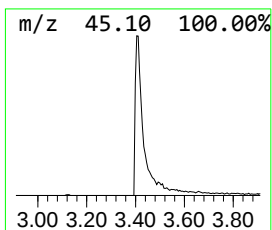
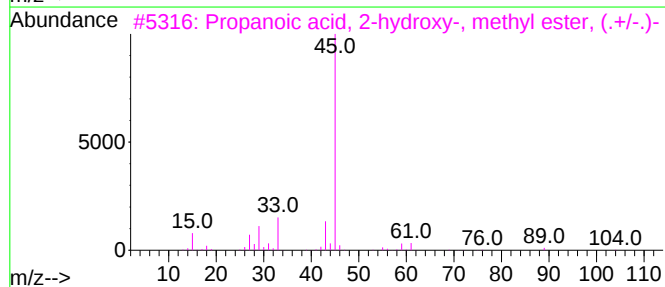
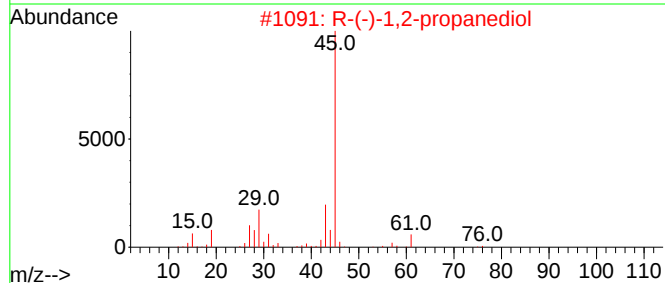
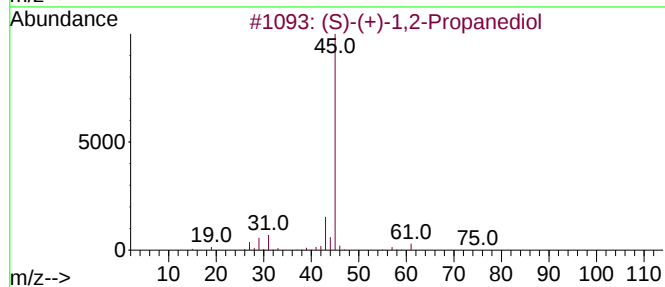
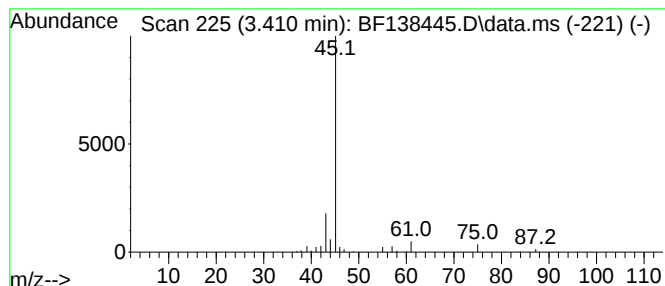
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.410	2.79 ng	130275	1,4-Dichlorobenzene-d4	6.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
3		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5		2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9



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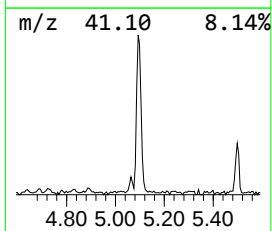
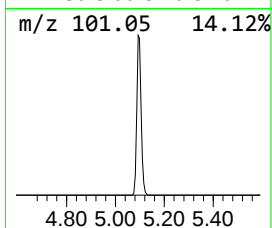
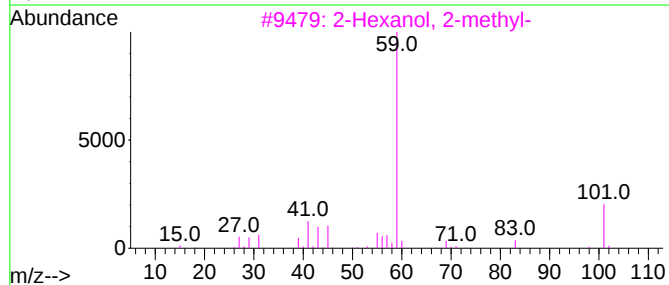
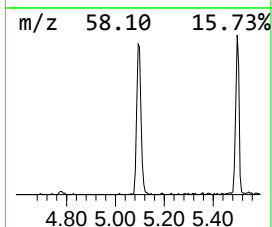
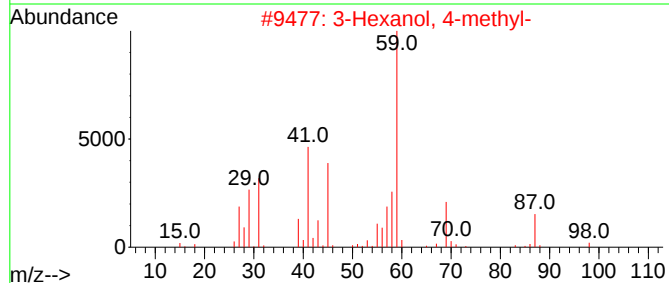
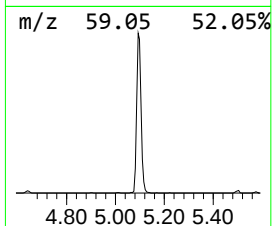
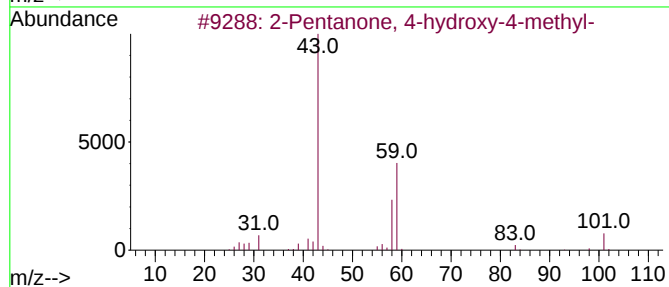
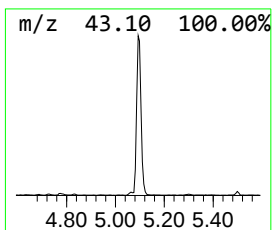
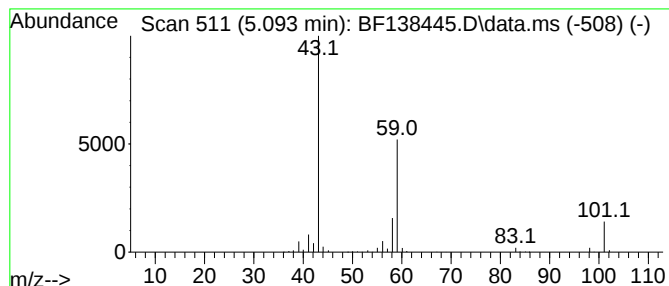
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.093	10.39 ng	485469	1,4-Dichlorobenzene-d4			6.869
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12



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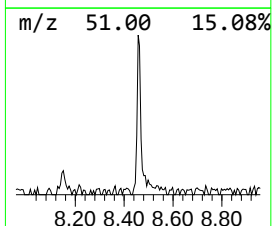
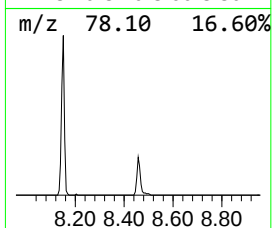
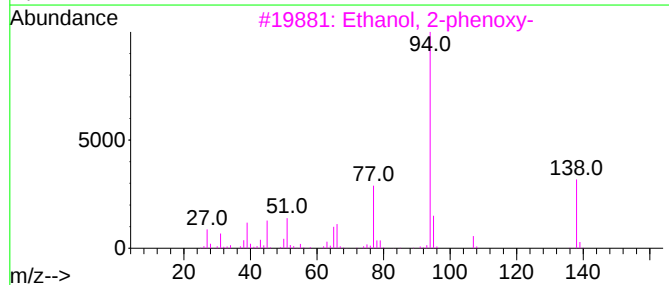
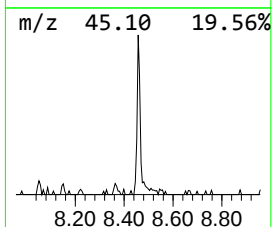
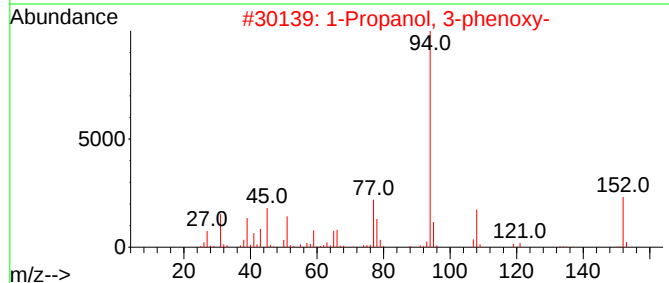
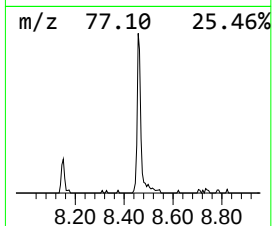
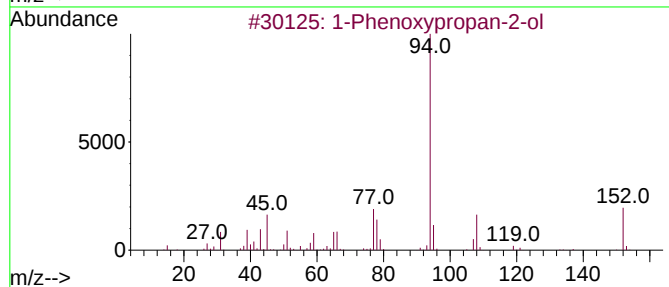
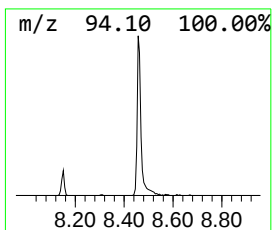
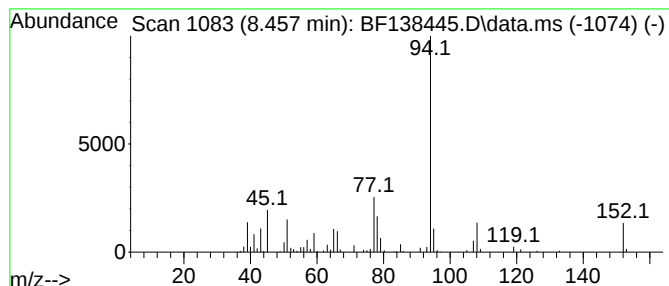
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.457	2.45 ng	148381	Naphthalene-d8	8.151

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	83
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	50
5		Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	47



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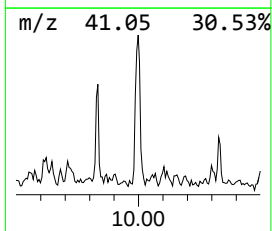
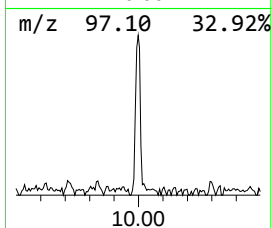
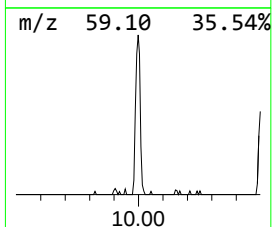
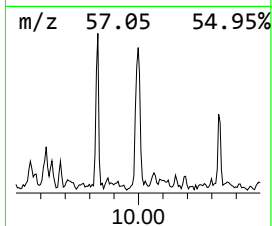
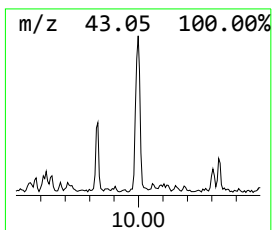
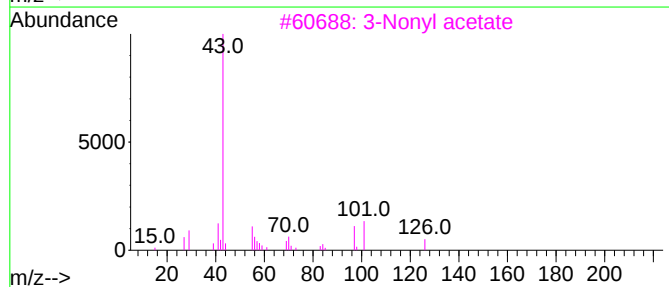
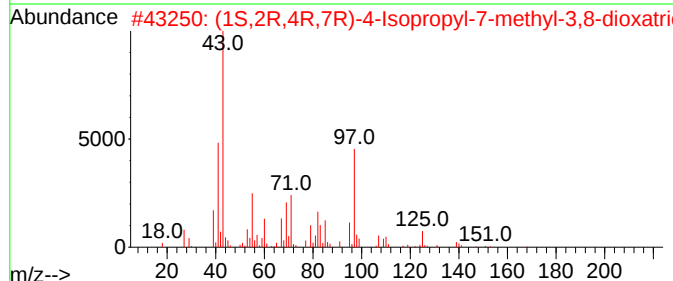
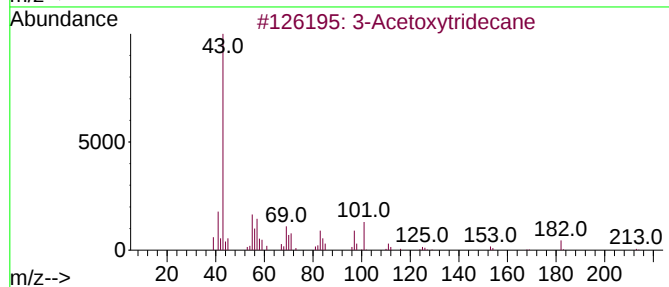
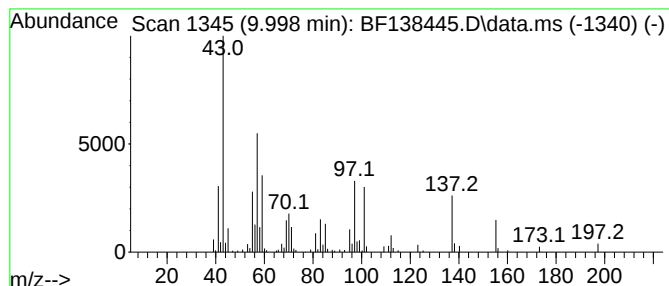
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown9.998 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.998	2.51 ng	167103	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Acetoxytridecane			242	C15H30O2	1010245-61-3	14
2	(1S,2R,4R,7R)-4-Isopropyl-7-meth...			168	C10H16O2	001619-26-7	14
3	3-Nonyl acetate			186	C11H22O2	1010429-16-2	12
4	Carbonic acid, octadecyl prop-1-...			354	C22H42O3	1000383-11-5	10
5	2-t-Butyl-5-propyl-[1,3]dioxolan...			186	C10H18O3	157733-17-0	10



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B-129-SB01

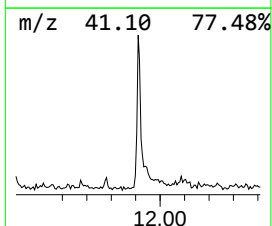
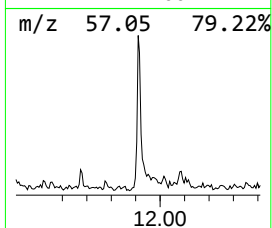
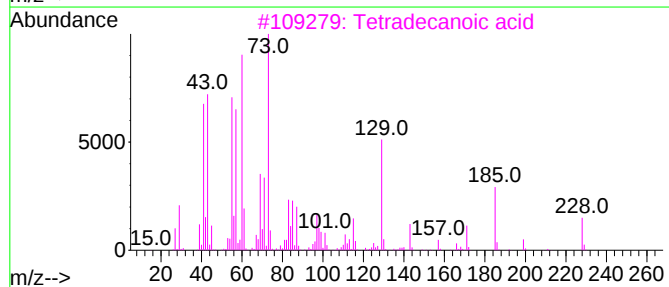
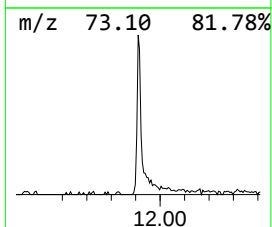
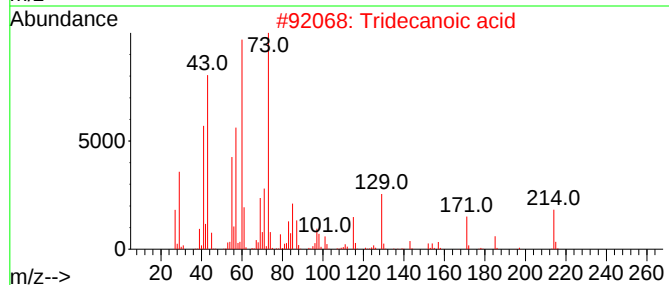
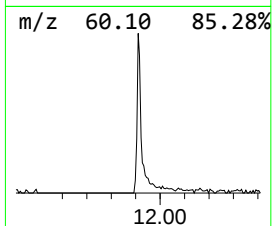
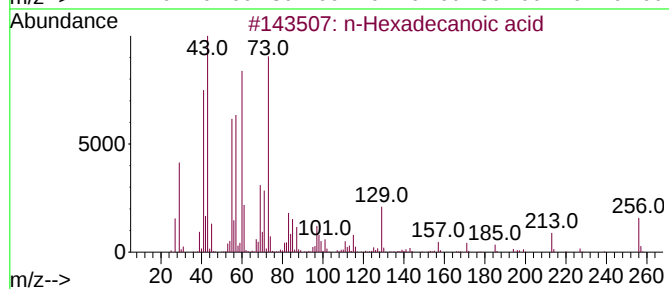
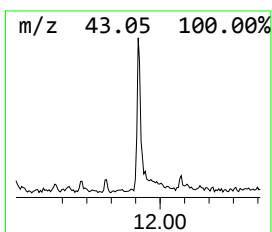
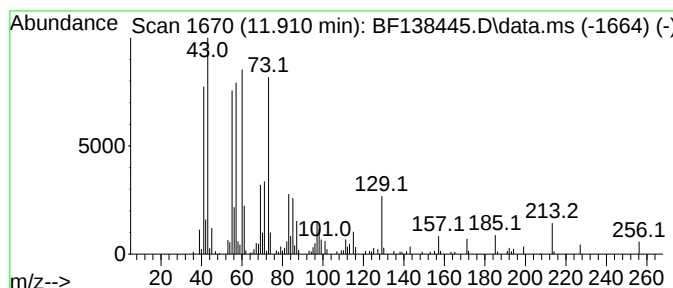
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.98 ng	219023	Phenanthrene-d10	11.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2		Tridecanoic acid	214	C13H26O2	000638-53-9	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138445.D
Acq On : 03 Jul 2024 14:44
Operator : CG\JU
Sample : P3141-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-129-SB01

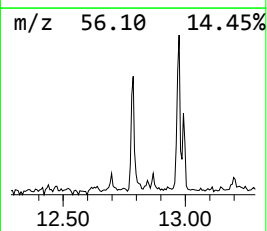
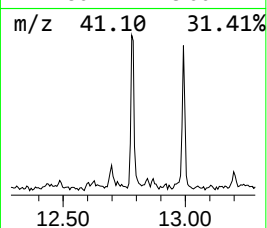
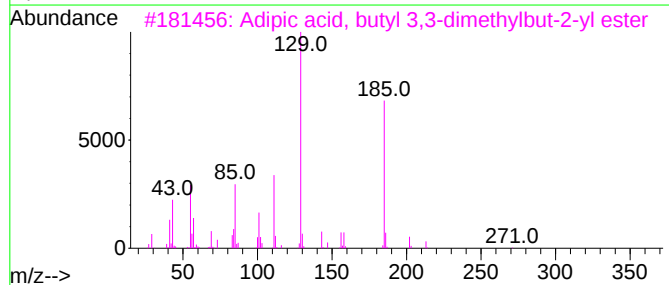
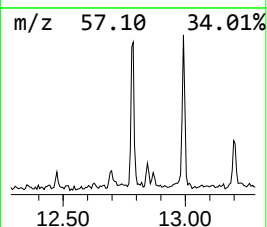
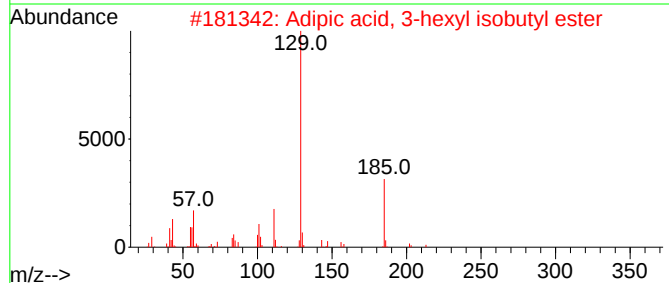
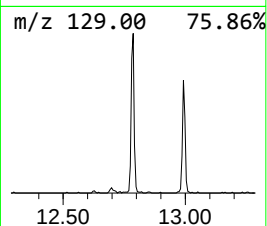
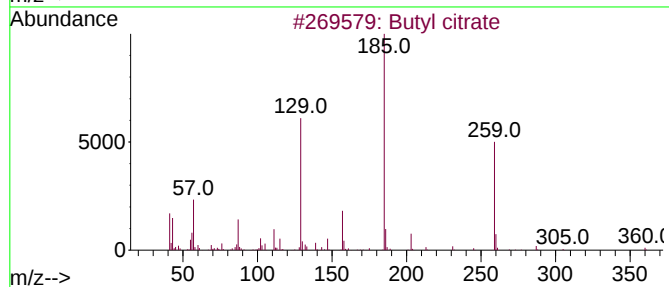
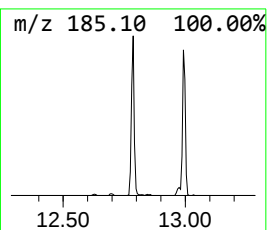
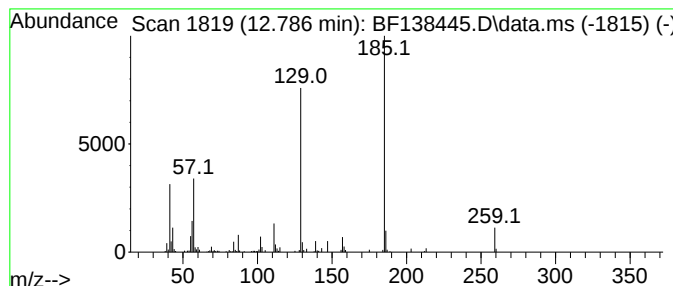
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Butyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	3.87 ng	157476	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	78
2			Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	78
3			Adipic acid, butyl 3,3-dimethylb...	286	C16H30O4	1000353-66-8	72
4			Adipic acid, 2-heptyl isobutyl e...	300	C17H32O4	1000353-64-3	64
5			Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138445.D
Acq On : 03 Jul 2024 14:44
Operator : CG\JU
Sample : P3141-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-129-SB01

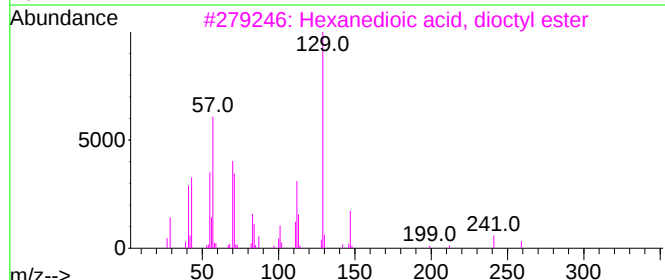
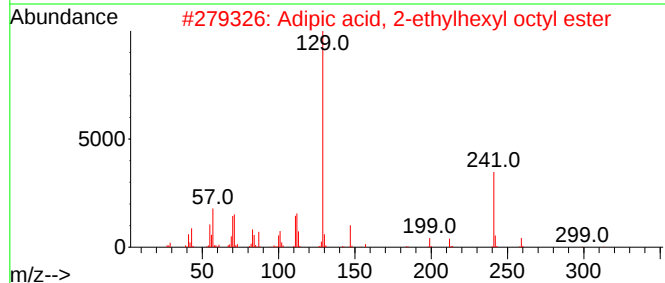
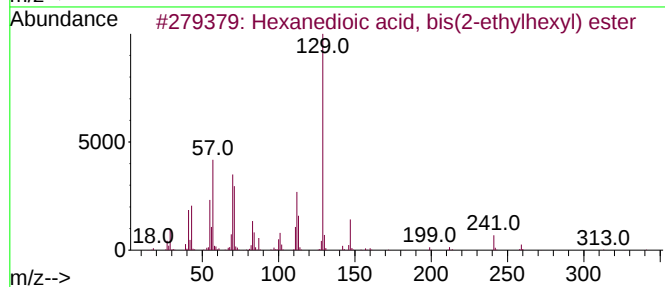
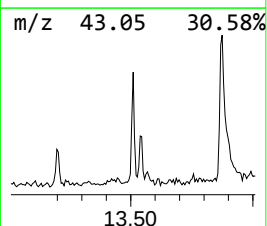
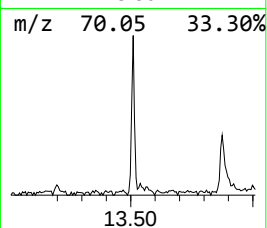
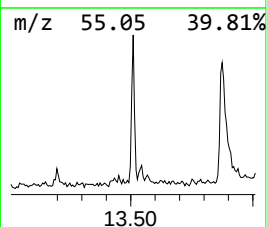
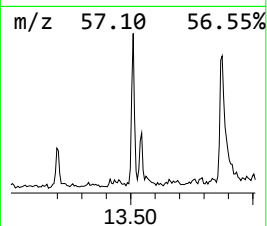
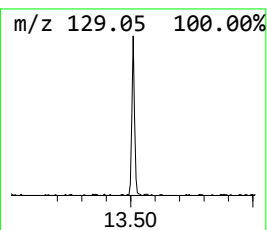
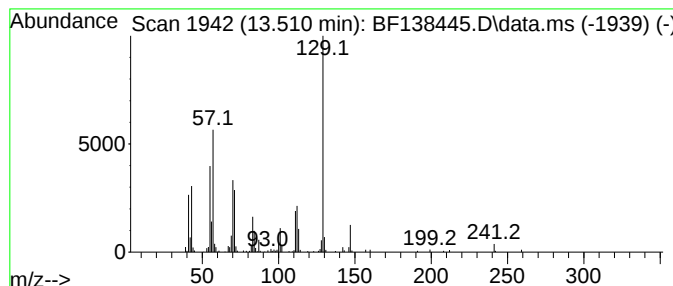
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.510	3.44 ng	140010	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
3			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	76
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	64
5			Diisooctyl adipate	370	C22H42O4	001330-86-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138445.D
Acq On : 03 Jul 2024 14:44
Operator : CG\JU
Sample : P3141-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-129-SB01

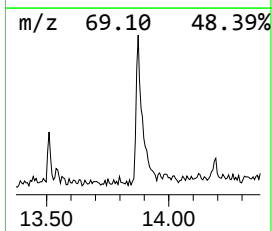
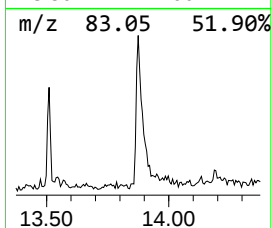
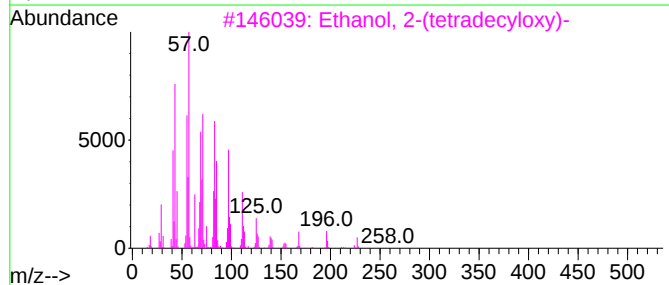
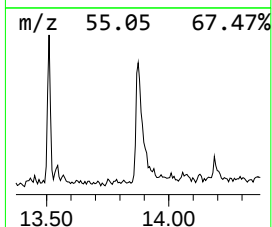
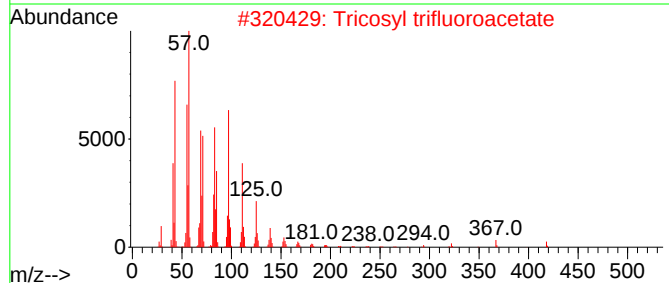
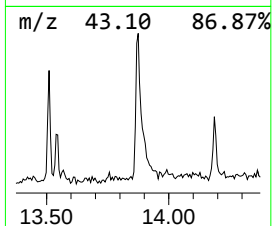
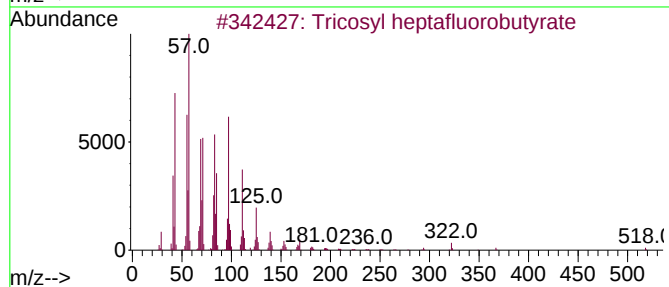
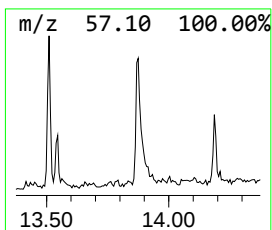
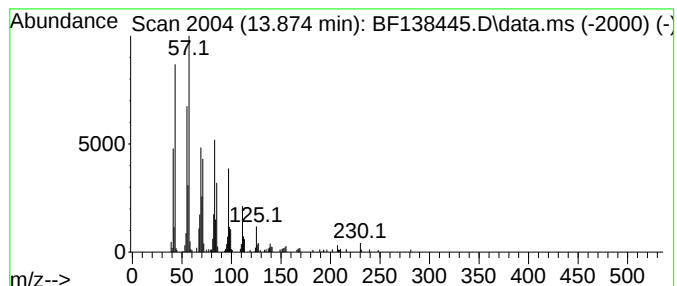
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tricosyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.85 ng	238154	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
2			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138445.D
Acq On : 03 Jul 2024 14:44
Operator : CG\JU
Sample : P3141-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-129-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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(S)-(+)-1,2-Pro...	3.410	2.8	ng	130275	1	6.869	934558	20.0
2-Pentanone, 4-...	5.093	10.4	ng	485469	1	6.869	934558	20.0
1-Phenoxypropan...	8.457	2.5	ng	148381	2	8.151	1213360	20.0
unknown9.998	9.998	2.5	ng	167103	3	9.904	1333060	20.0
n-Hexadecanoic ...	11.910	4.0	ng	219023	4	11.392	1099440	20.0
Butyl citrate	12.786	3.9	ng	157476	5	14.027	814520	20.0
Hexanedioic aci...	13.510	3.4	ng	140010	5	14.027	814520	20.0
Tricosyl heptaf...	13.874	5.8	ng	238154	5	14.027	814520	20.0