LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070324\
Data File : BF138444.D
Acq On : 03 Jul 2024 14:15
Operator : CG\JU
Sample : P3141-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-140-SB02

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: BF138444.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	10	18	24	rBV	2746305	3620821	92.10%	12.152%
2	2.299	32	36	41	rBV	43849	53960	1.37%	0.181%
3	3.416	222	226	238	rBV	76968	148161	3.77%	0.497%
4	5.098	508	512	519	rVB	394774	487850	12.41%	1.637%
5	5.504	576	581	584	rBV	3965322	3748381	95.34%	12.580%
6	6.504	746	751	754	rBV	3408502	3633079	92.41%	12.193%
7	6.869	809	813	817	rBV	1148939	924633	23.52%	3.103%
8	7.434	903	909	912	rBV	2496143	2322140	59.06%	7.793%
9	7.681	948	951	955	rVB	108610	85462	2.17%	0.287%
10	8.151	1023	1031	1034	rBV	1477703	1221981	31.08%	4.101%
11	8.457	1073	1083	1091	rBV	120381	149743	3.81%	0.503%
12	8.739	1127	1131	1135	rVB	68146	57720	1.47%	0.194%
13	9.228	1208	1214	1217	rBV	4521029	3931569	100.00%	13.195%
14	9.304	1223	1227	1229	rBV	65053	57221	1.46%	0.192%
15	9.904	1325	1329	1332	rBV	1655943	1346395	34.25%	4.519%
16	9.998	1340	1345	1351	rBV2	163558	214970	5.47%	0.721%
17	10.692	1459	1463	1466	rBV	2243961	1955800	49.75%	6.564%
18	11.392	1578	1582	1584	rBV	1224337	1110215	28.24%	3.726%
19	11.910	1663	1670	1675	rBV	157895	181583	4.62%	0.609%
20	12.698	1800	1804	1809	rBV2	33629	43419	1.10%	0.146%
21	12.974	1847	1851	1854	rBV	3072062	2578628	65.59%	8.654%
22	13.868	2000	2003	2021	rBV	179321	300111	7.63%	1.007%
23	14.027	2026	2030	2033	rBV	862322	792957	20.17%	2.661%
24	14.492	2106	2109	2111	rBV	65966	61510	1.56%	0.206%
25	15.139	2215	2219	2223	rVB	52476	56595	1.44%	0.190%
26	15.492	2274	2279	2292	rBV	557492	710980	18.08%	2.386%

Sum of corrected areas: 29795884

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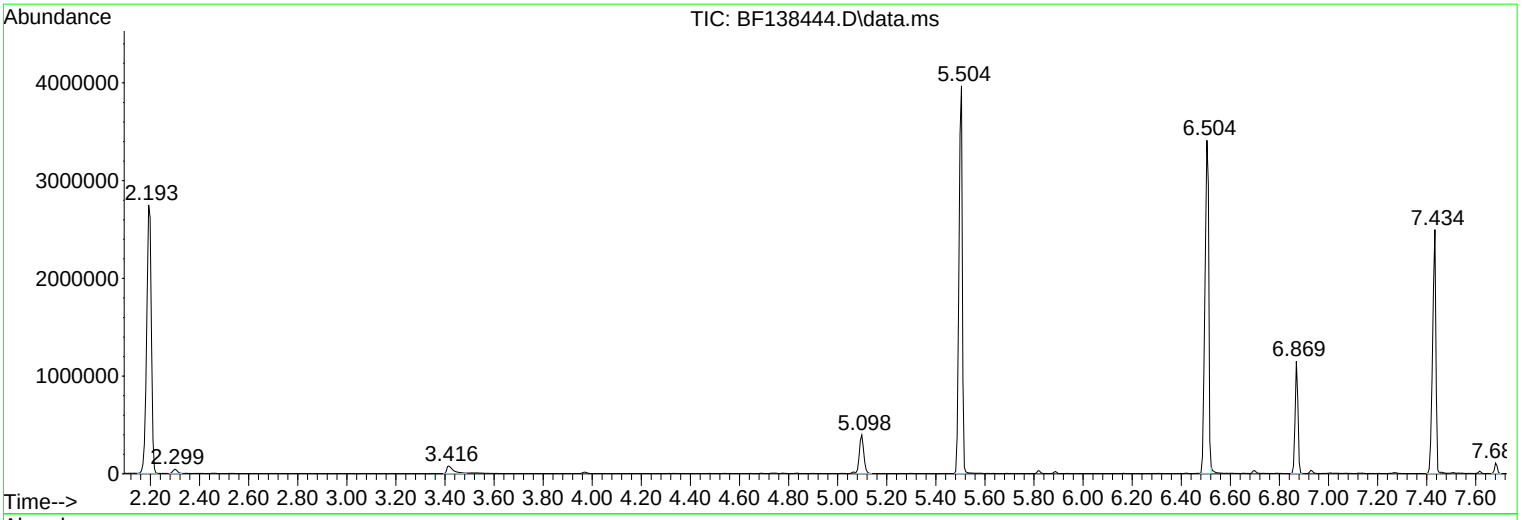
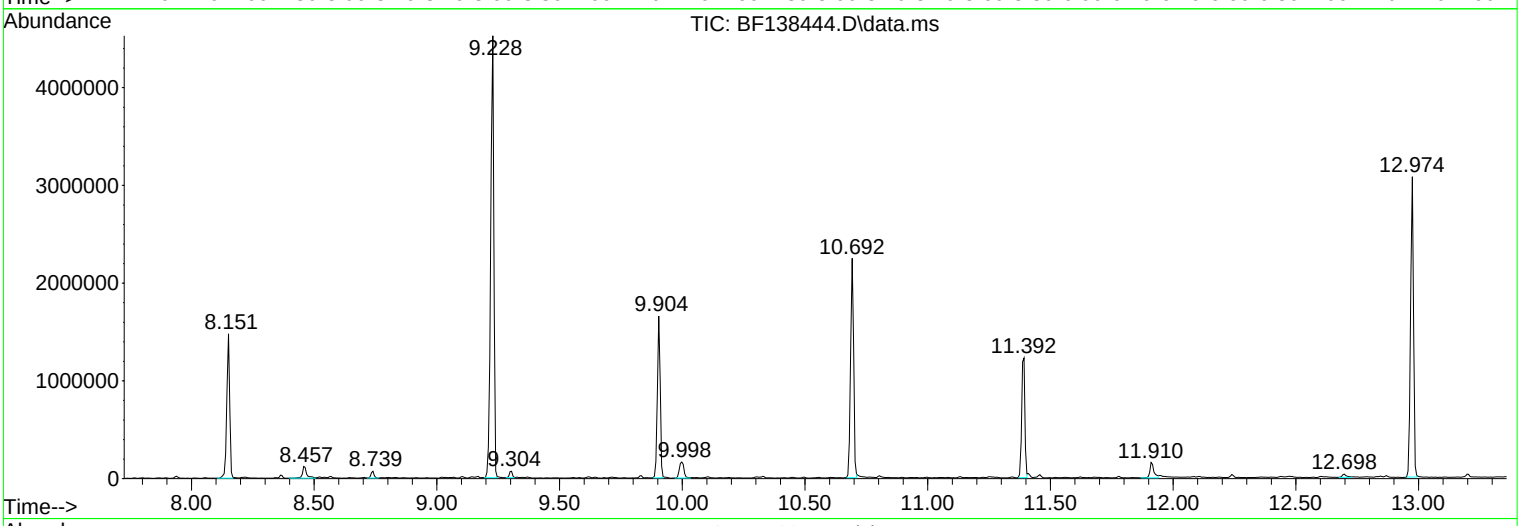
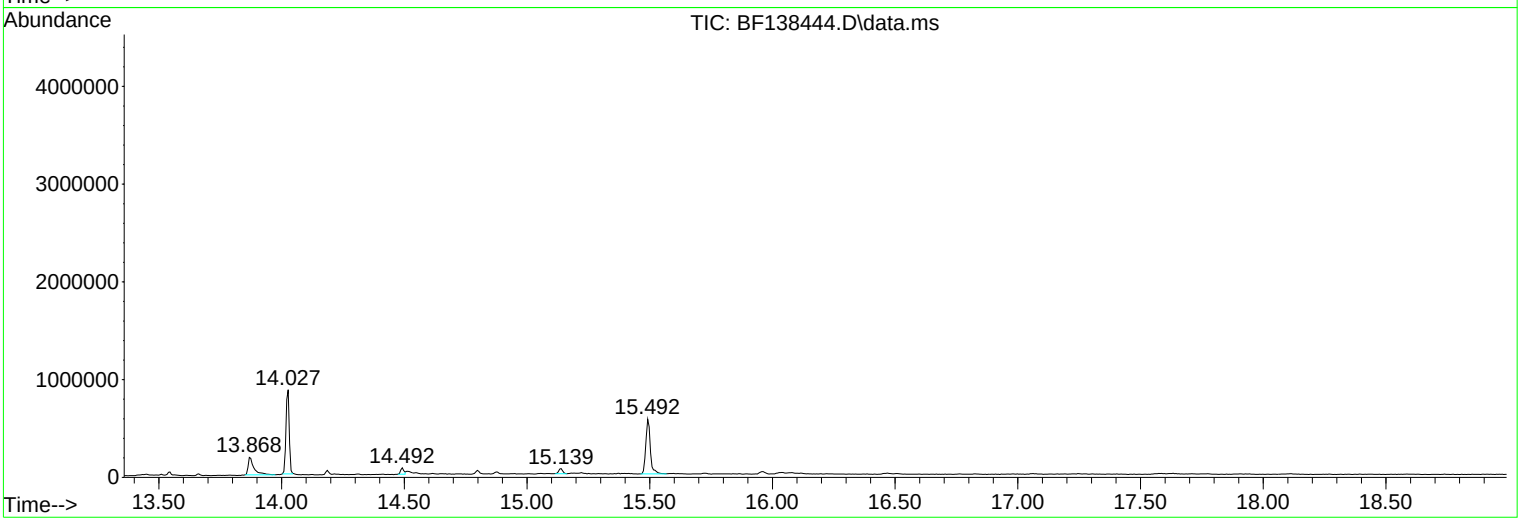
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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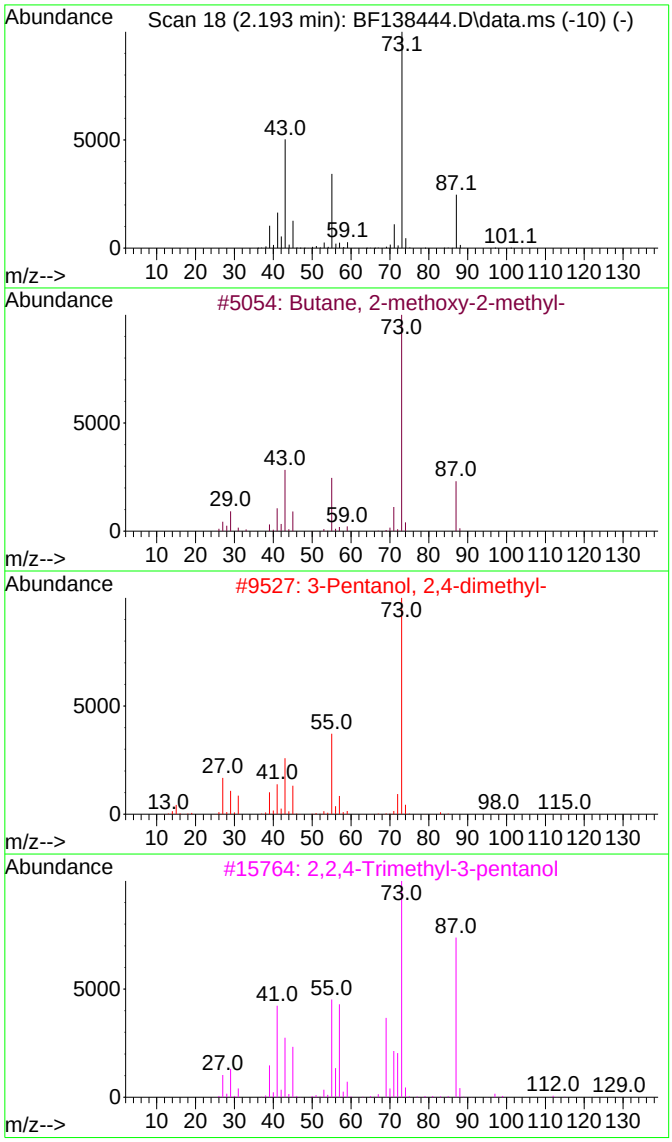
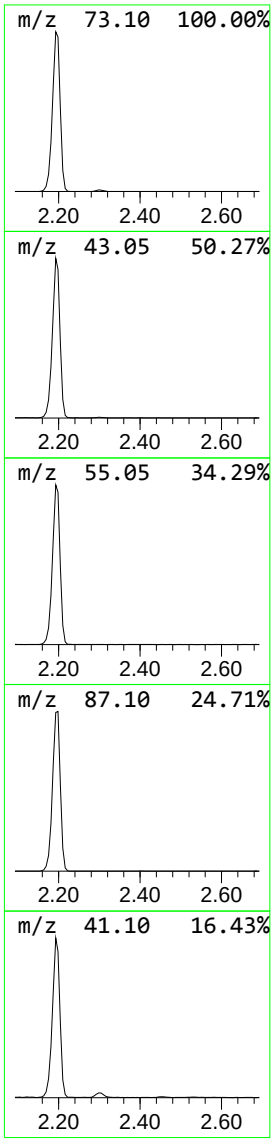
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	78.32 ng	3620820	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	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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B-140-SB02

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

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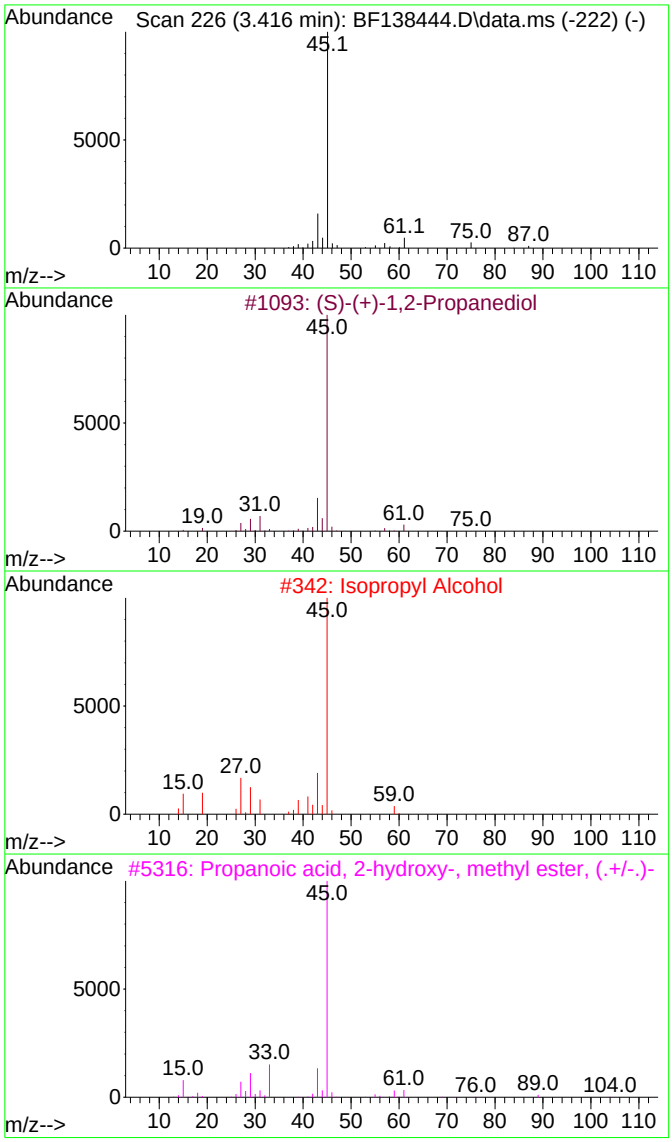
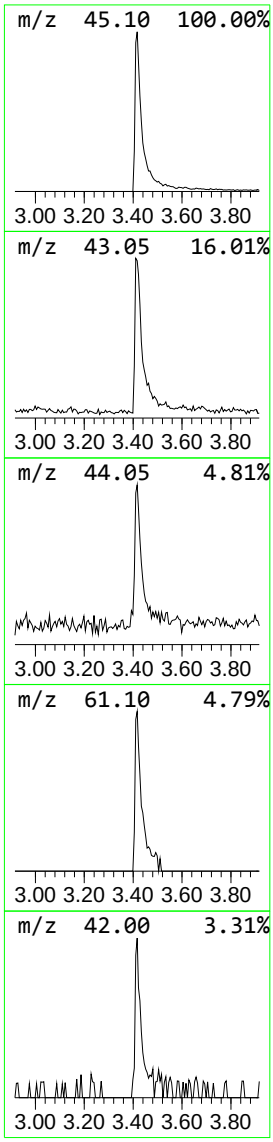
Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.416	3.20 ng	148161	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	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4	Trimethylene glycol monomethyl e...	90	C4H10O2	001589-49-7	9
5	Propylene Glycol	76	C3H8O2	000057-55-6	9





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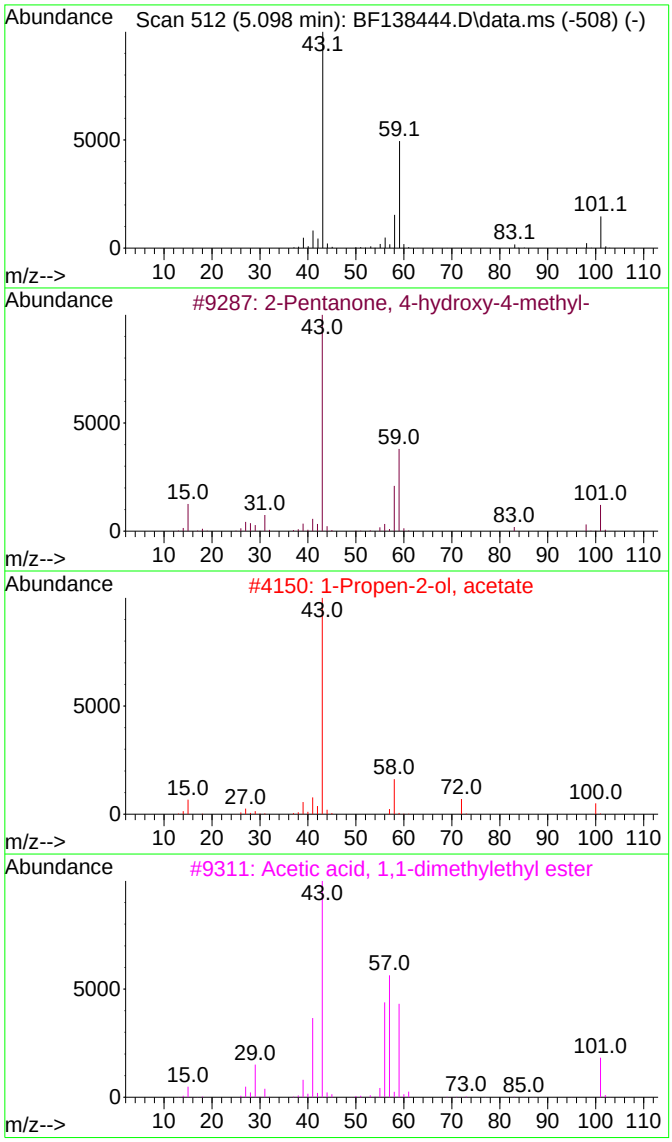
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

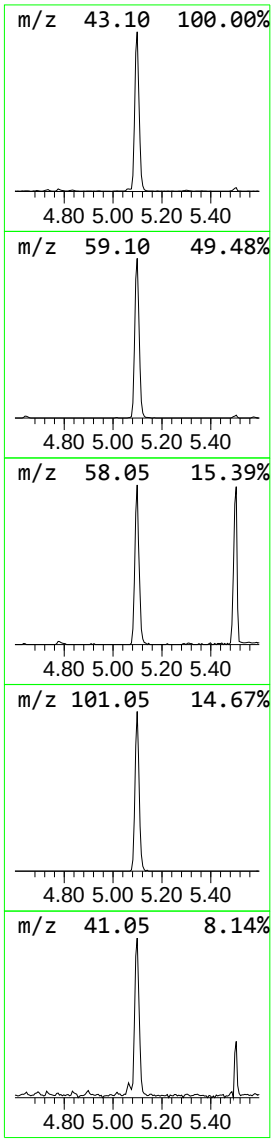
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	10.55 ng	487850	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	59
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	Acetone	58	C3H6O	000067-64-1	7





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
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TIC Library : C:\Database\NIST20.L
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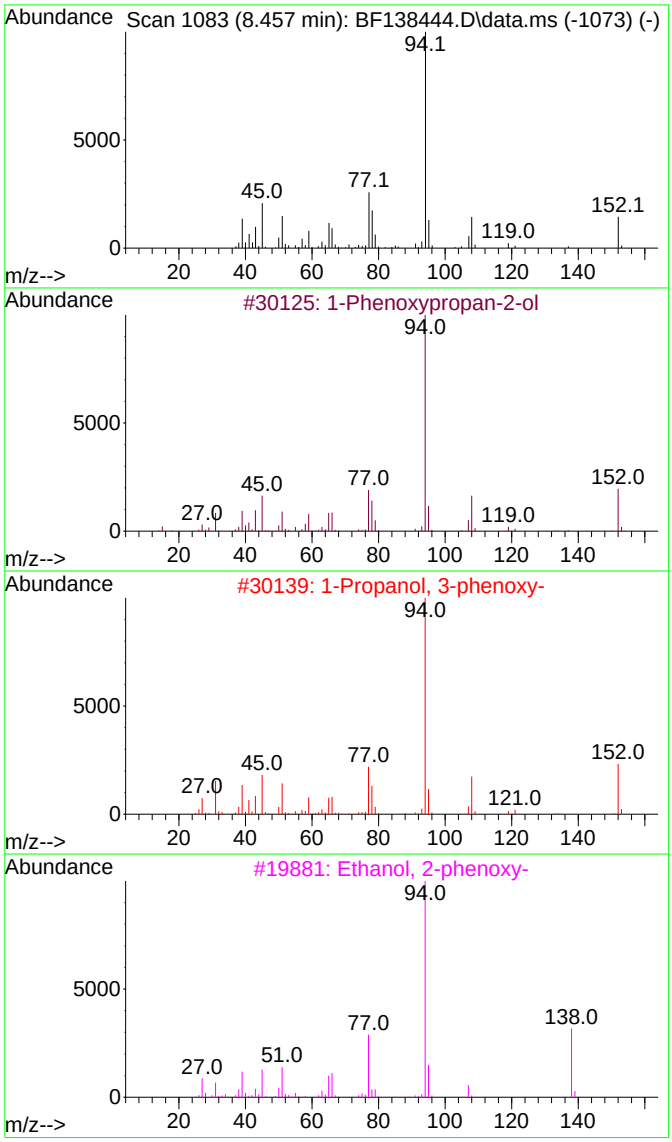
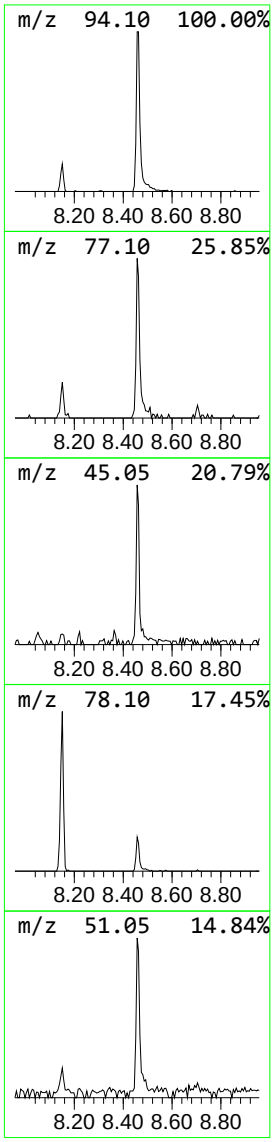
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.457	2.45 ng	149743	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	72
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	50
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	50





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Instrument :
BNA_F
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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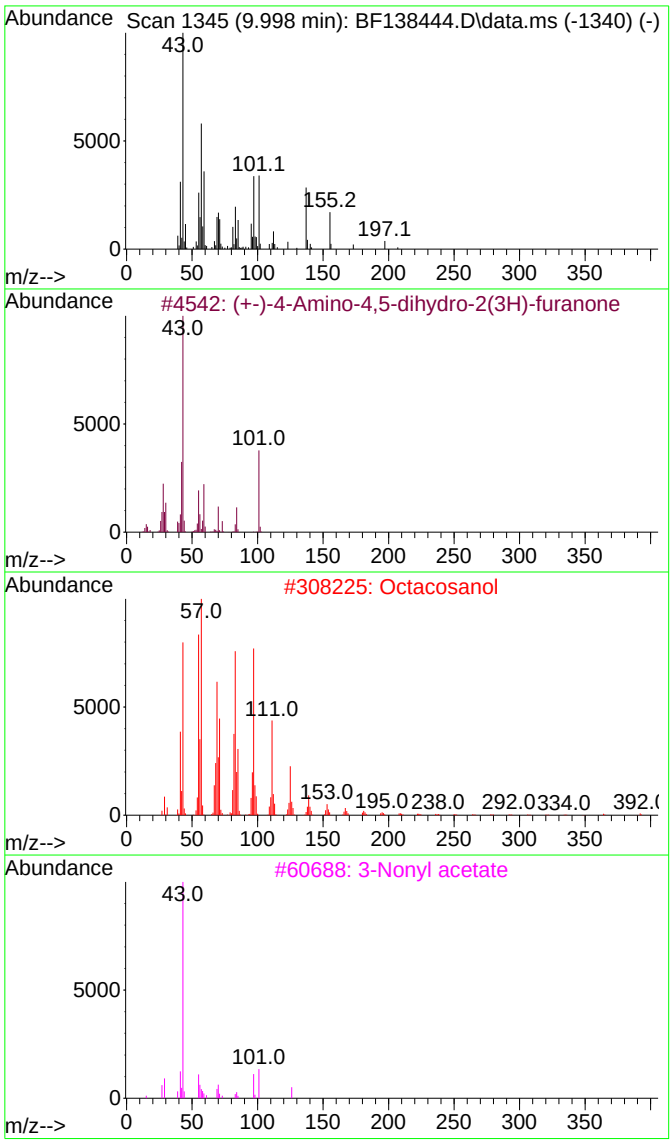
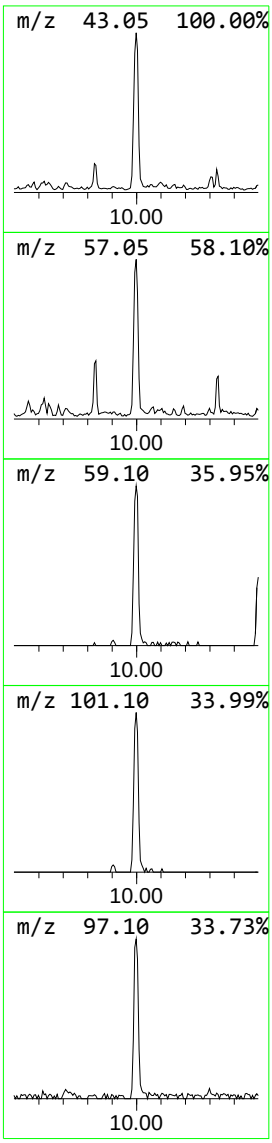
Peak Number 5 unknown9.998 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.998	3.19 ng	214970	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	22
2	Octacosanol	410	C28H58O	000557-61-9	22
3	3-Nonyl acetate	186	C11H22O2	1010429-16-2	22
4	Triacontyl acetate	480	C32H64O2	041755-58-2	22
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	22





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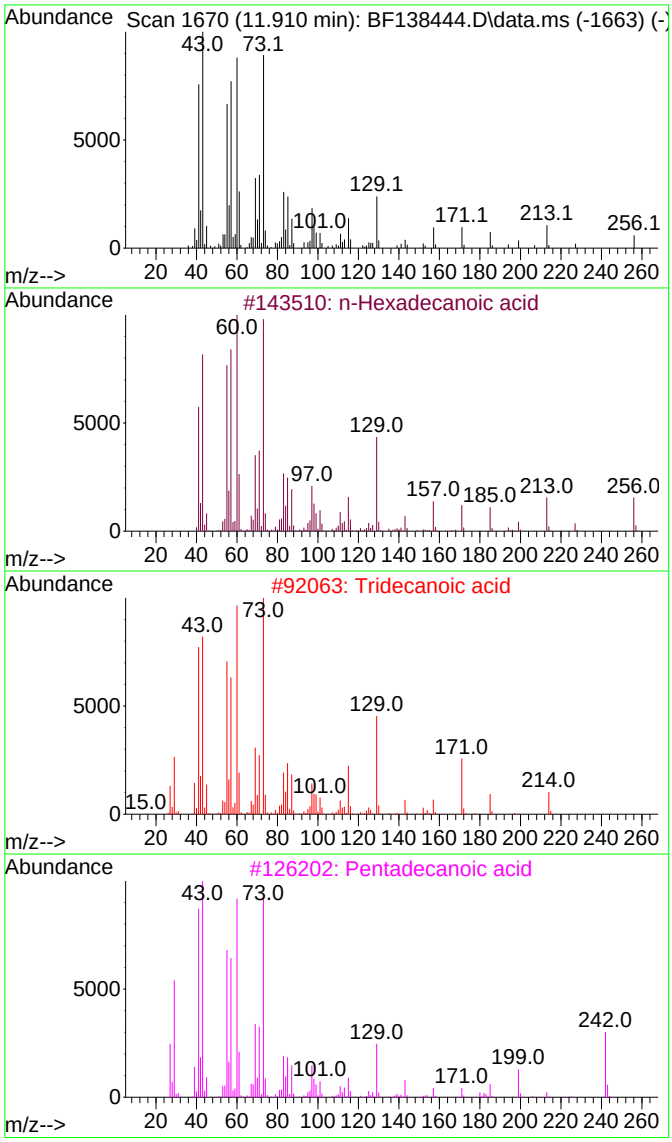
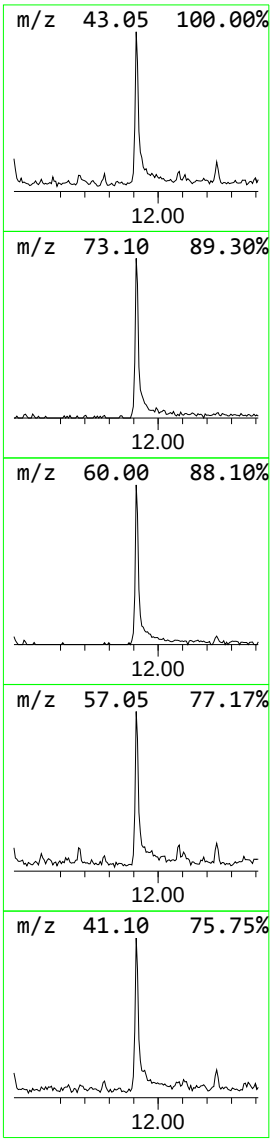
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.27 ng	181583	Phenanthrene-d10	11.392

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59





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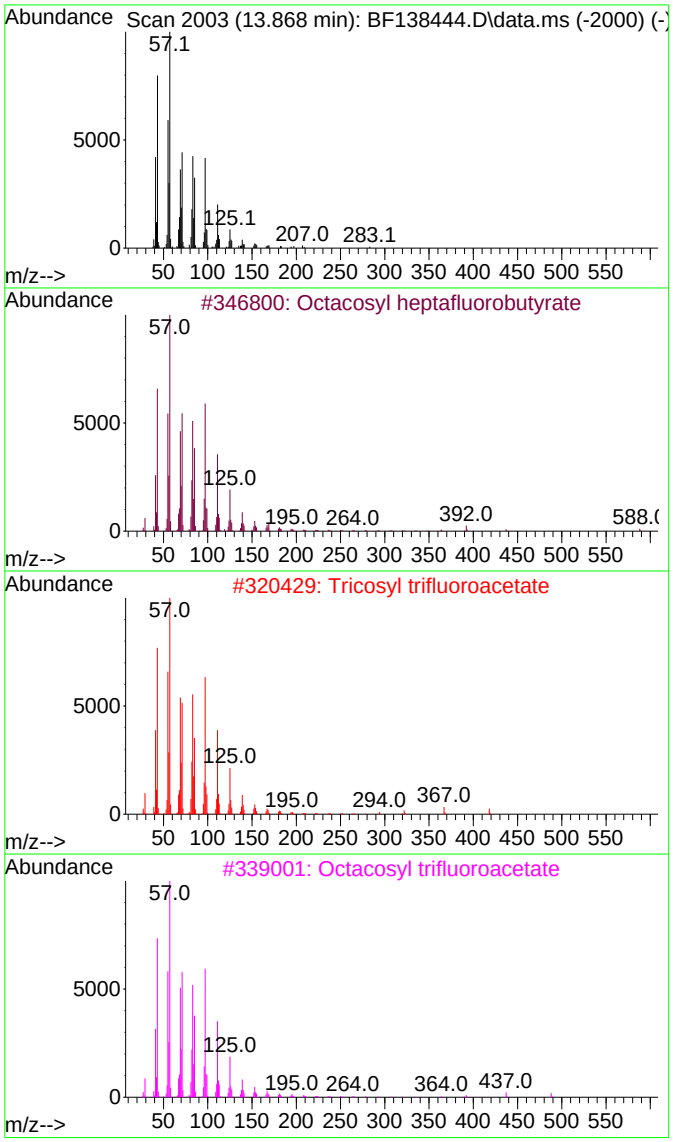
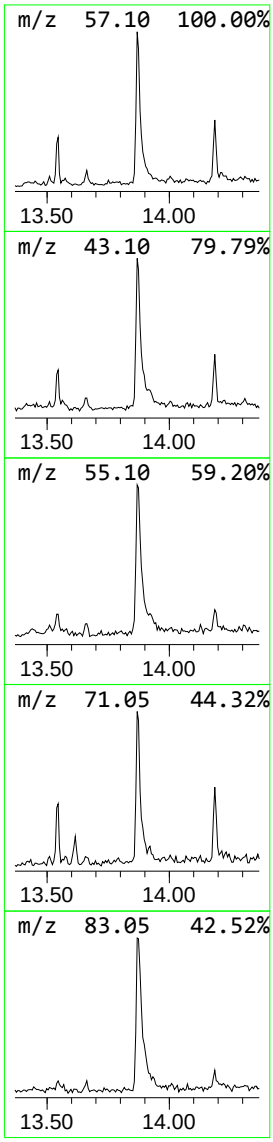
****

Peak Number 7 Octacosyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	7.57 ng	300111	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	91
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
5	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.193	78.3	ng	3620820	1	6.869	924633	20.0
(S)-(+)-1,2-Pro...	3.416	3.2	ng	148161	1	6.869	924633	20.0
2-Pentanone, 4-...	5.098	10.6	ng	487850	1	6.869	924633	20.0
1-Phenoxypropan...	8.457	2.5	ng	149743	2	8.151	1221980	20.0
unknown9.998	9.998	3.2	ng	214970	3	9.904	1346400	20.0
n-Hexadecanoic ...	11.910	3.3	ng	181583	4	11.392	1110220	20.0
Octacosyl hepta...	13.868	7.6	ng	300111	5	14.027	792957	20.0