LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071224\
Data File : BF138548.D
Acq On : 12 Jul 2024 16:03
Operator : CG\JU
Sample : P3193-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-2

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138548.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	6	14	21	rVB	1558502	2033968	87.50%	12.127%
2	3.393	220	222	235	rBV	28131	68308	2.94%	0.407%
3	5.087	507	510	518	rVB	132644	154026	6.63%	0.918%
4	5.492	575	579	582	rBV	2221387	1944204	83.63%	11.592%
5	6.498	745	750	753	rBV	2206263	1997419	85.92%	11.909%
6	6.692	780	783	792	rBV	22173	25891	1.11%	0.154%
7	6.863	808	812	815	rBV	737341	554944	23.87%	3.309%
8	7.428	903	908	911	rBV	1492358	1325252	57.01%	7.901%
9	7.675	946	950	957	rBV	49413	42509	1.83%	0.253%
10	8.145	1025	1030	1033	rBV	897400	730061	31.41%	4.353%
11	8.451	1079	1082	1093	rBV	88325	91626	3.94%	0.546%
12	9.222	1207	1213	1216	rBV	2661636	2324641	100.00%	13.860%
13	9.898	1324	1328	1331	rBV	1018343	801358	34.47%	4.778%
14	9.992	1339	1344	1348	rVB2	61069	74312	3.20%	0.443%
15	10.686	1458	1462	1465	rBV	1384753	1175078	50.55%	7.006%
16	11.380	1576	1580	1584	rBV	844074	674113	29.00%	4.019%
17	11.904	1665	1669	1677	rBV2	83897	93684	4.03%	0.559%
18	12.963	1845	1849	1853	rBV	1775816	1515615	65.20%	9.036%
19	13.863	1998	2002	2016	rBV2	64296	144276	6.21%	0.860%
20	14.015	2024	2028	2032	rBV	527022	453824	19.52%	2.706%
21	14.480	2103	2107	2110	rBV	33262	30394	1.31%	0.181%
22	14.862	2168	2172	2175	rBV	27690	27438	1.18%	0.164%
23	15.121	2213	2216	2221	rVB	34981	39250	1.69%	0.234%
24	15.480	2272	2277	2288	rBV	314672	410400	17.65%	2.447%
25	15.939	2351	2355	2361	rVB2	26922	40077	1.72%	0.239%

Sum of corrected areas: 16772668

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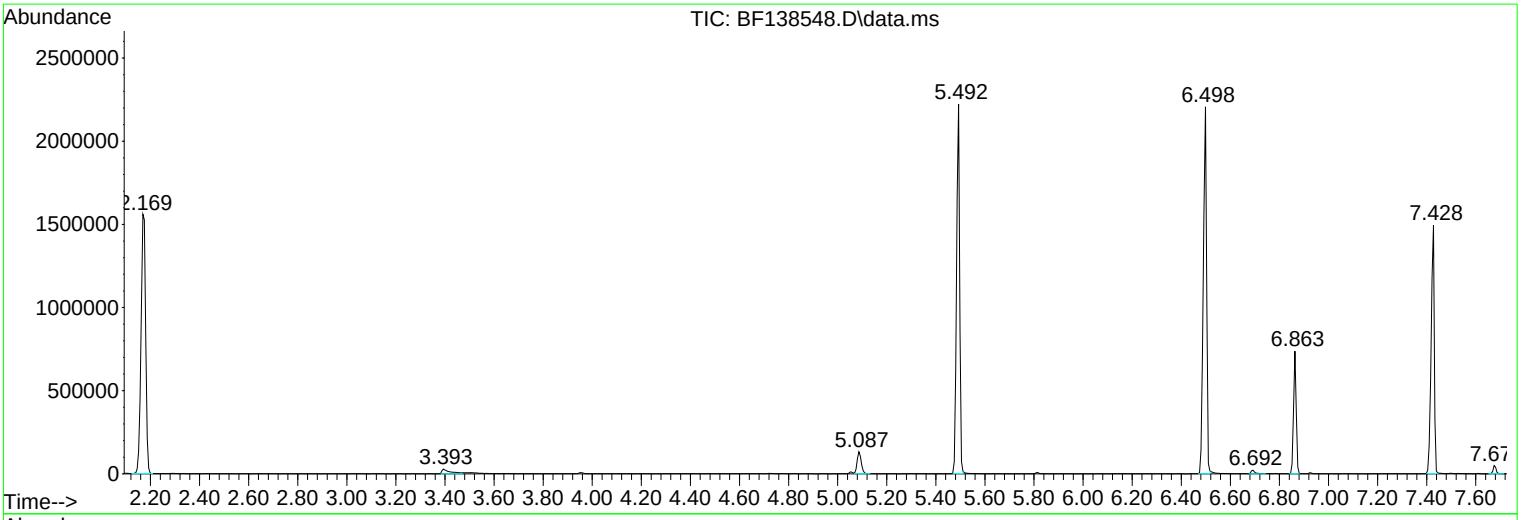
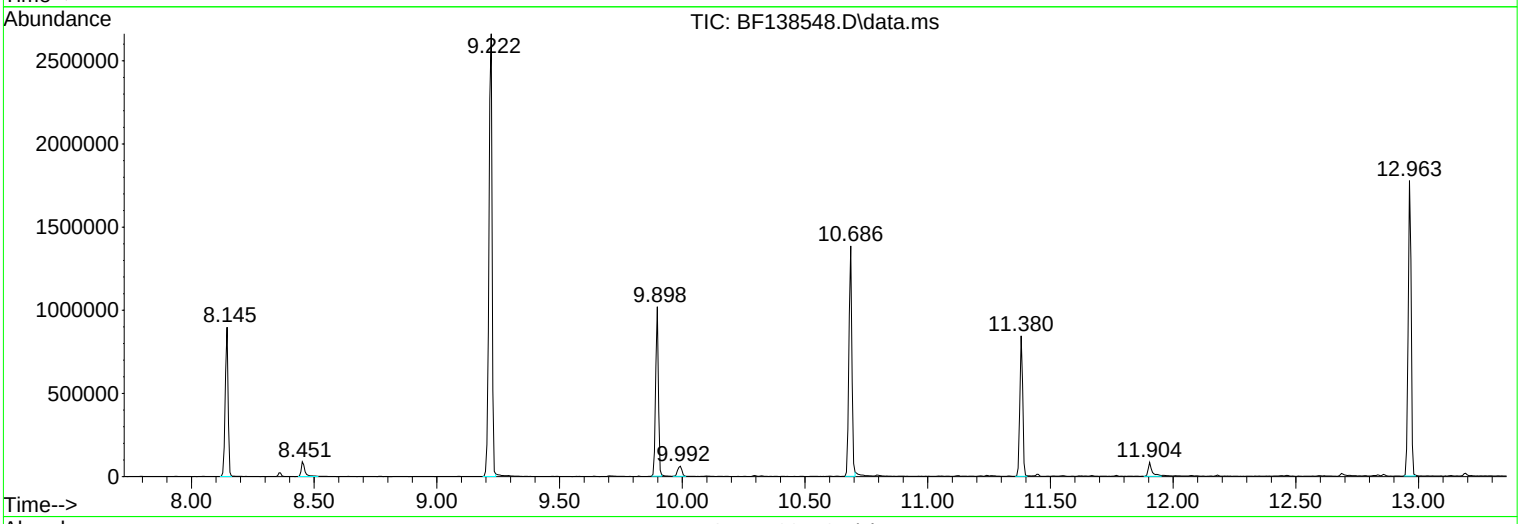
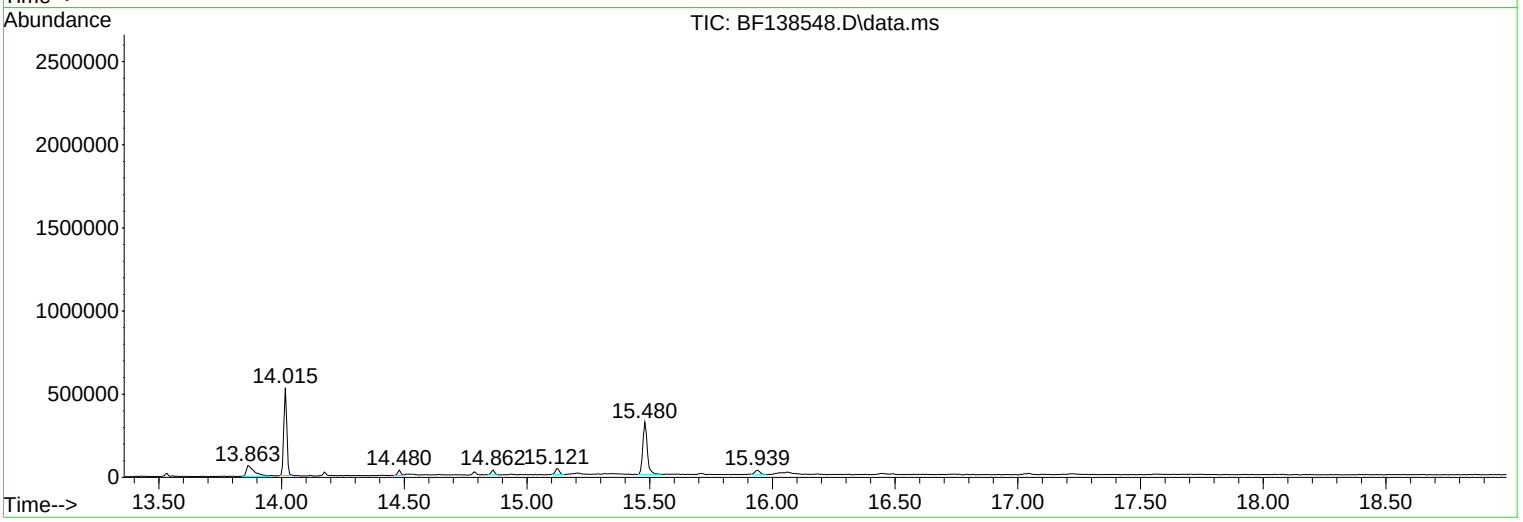
ClientSampleId :
FILL-MATERIAL-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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BNA_F
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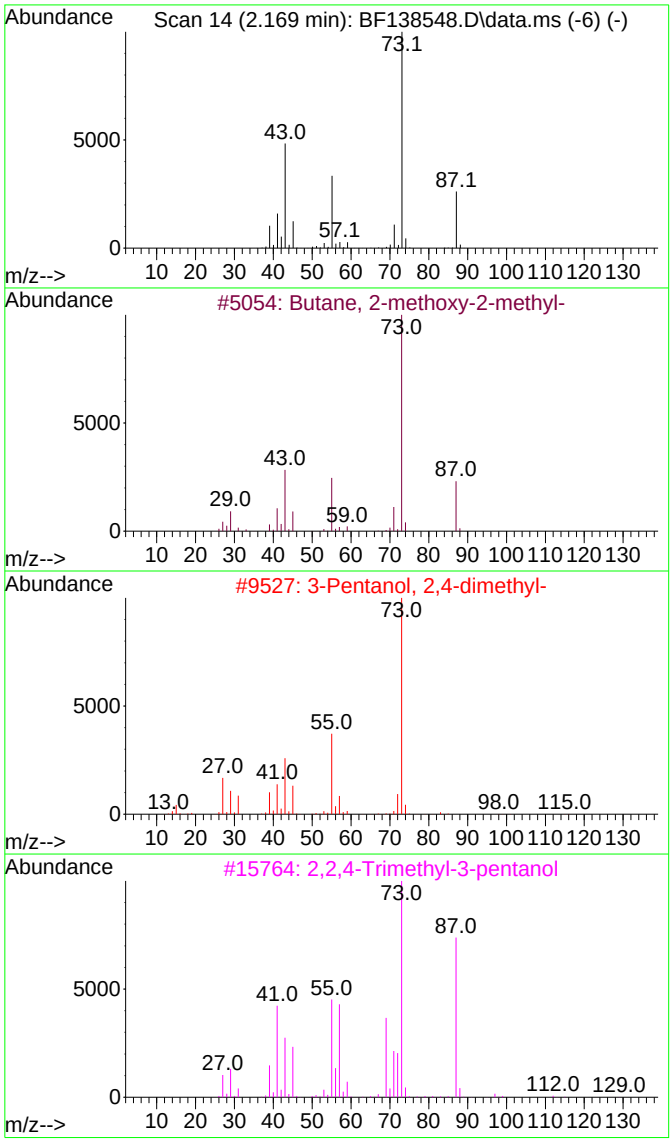
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

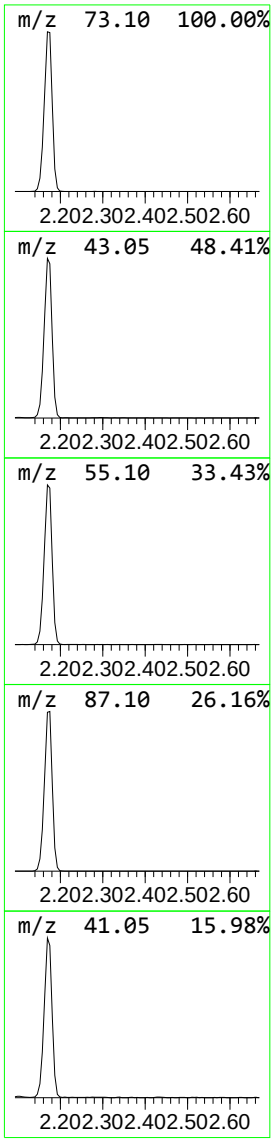
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	73.30 ng	2033970	1,4-Dichlorobenzene-d4	6.863

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23





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Data File : BF138548.D
Acq On : 12 Jul 2024 16:03
Operator : CG\JU
Sample : P3193-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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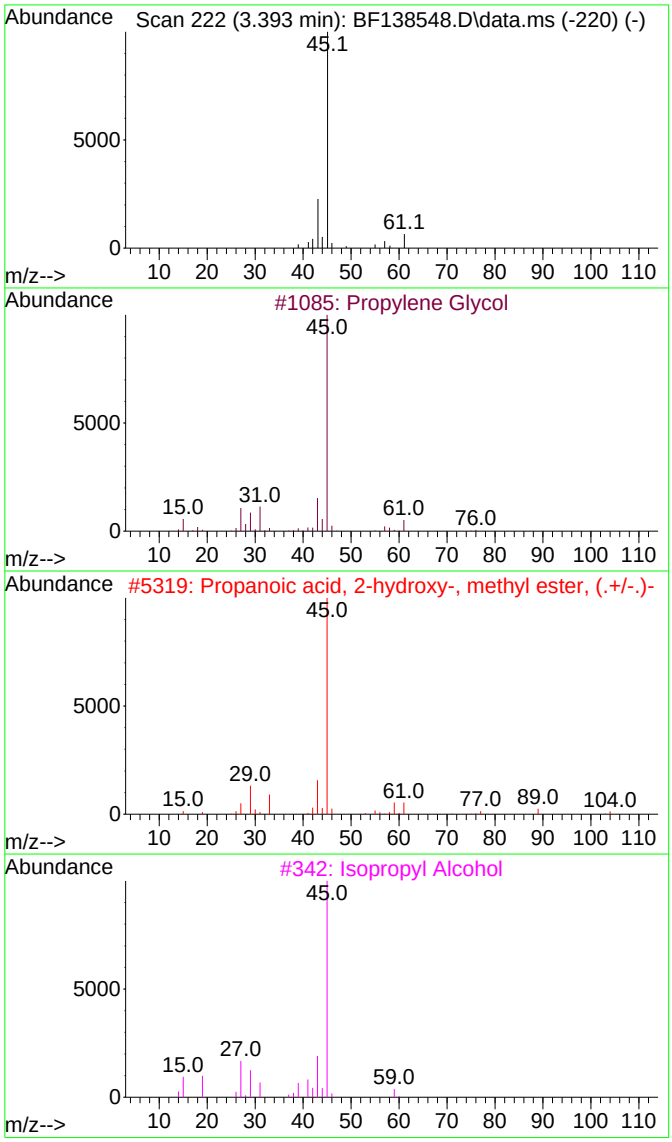
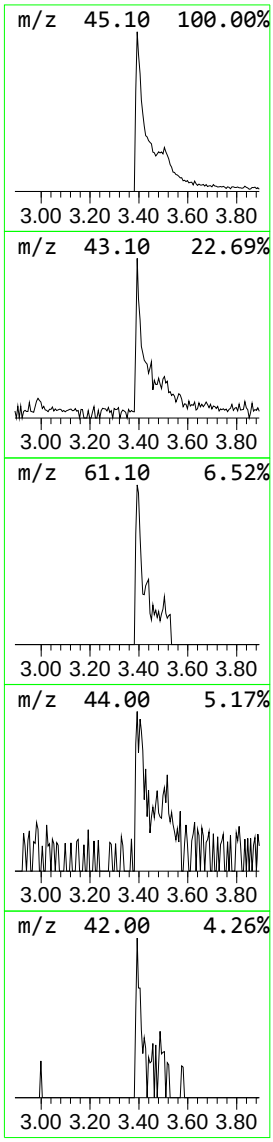
Peak Number 2 unknown3.393 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	2.46 ng	68308	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Formamide	45	CH3NO	000075-12-7	5
5	2-Butanol, 3-chloro-, (R*,R*)-	108	C4H9ClO	010325-40-3	4





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Data File : BF138548.D
Acq On : 12 Jul 2024 16:03
Operator : CG\JU
Sample : P3193-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-2

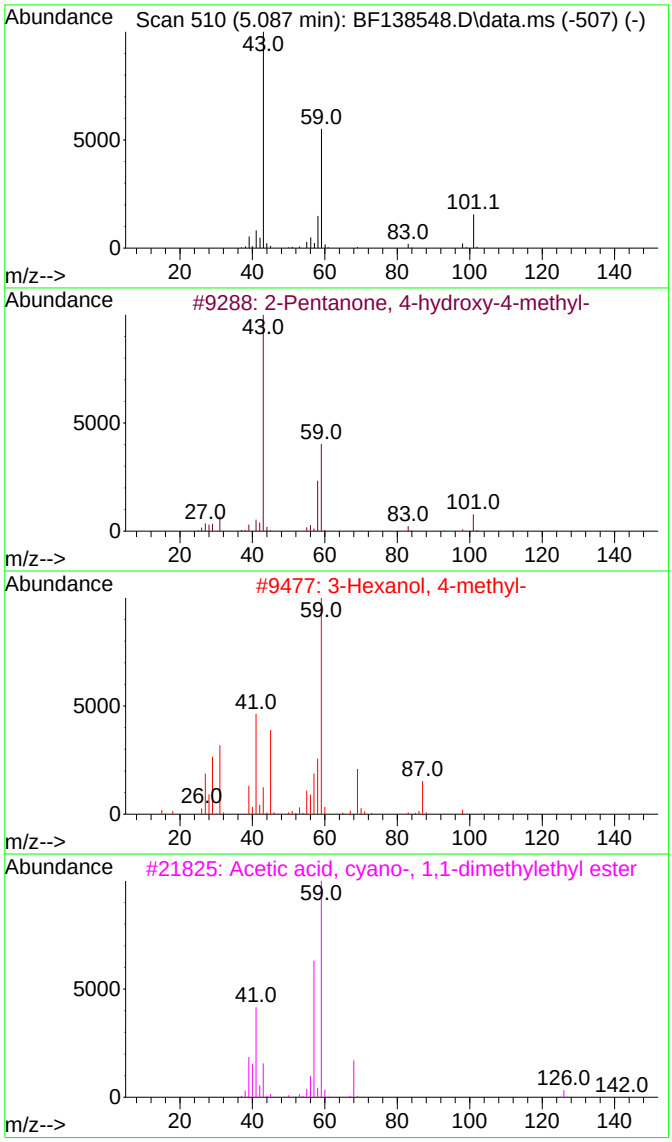
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

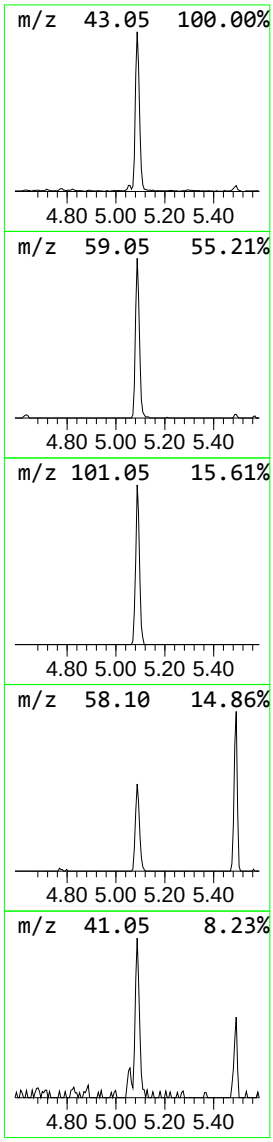
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	5.55 ng	154026	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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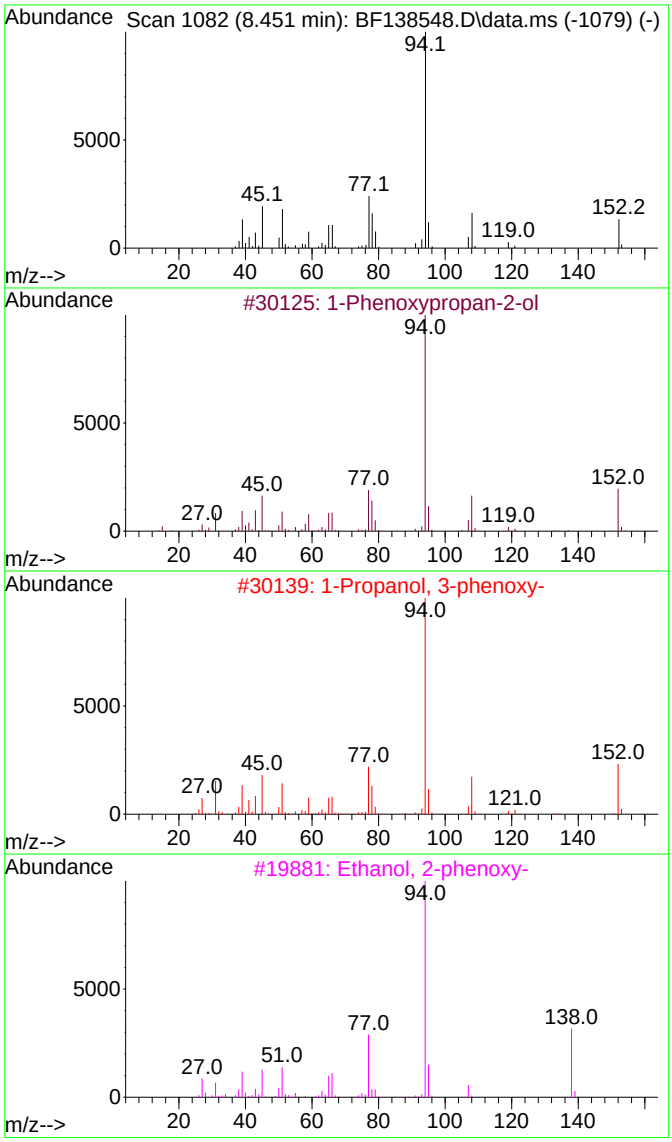
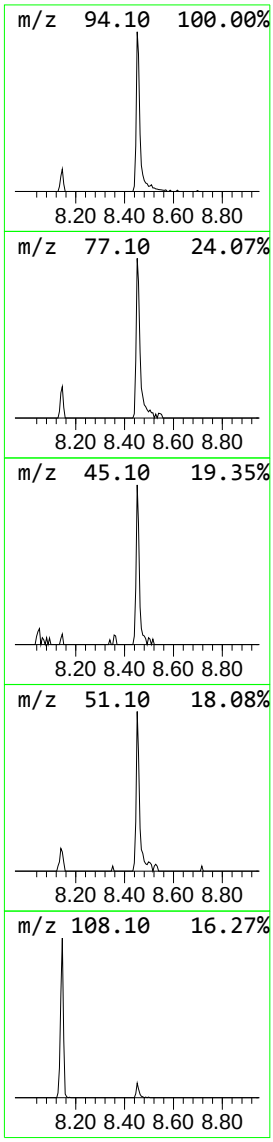
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	2.51 ng	91626	Naphthalene-d8	8.145

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	91
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	50
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	50





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Sample : P3193-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FILL-MATERIAL-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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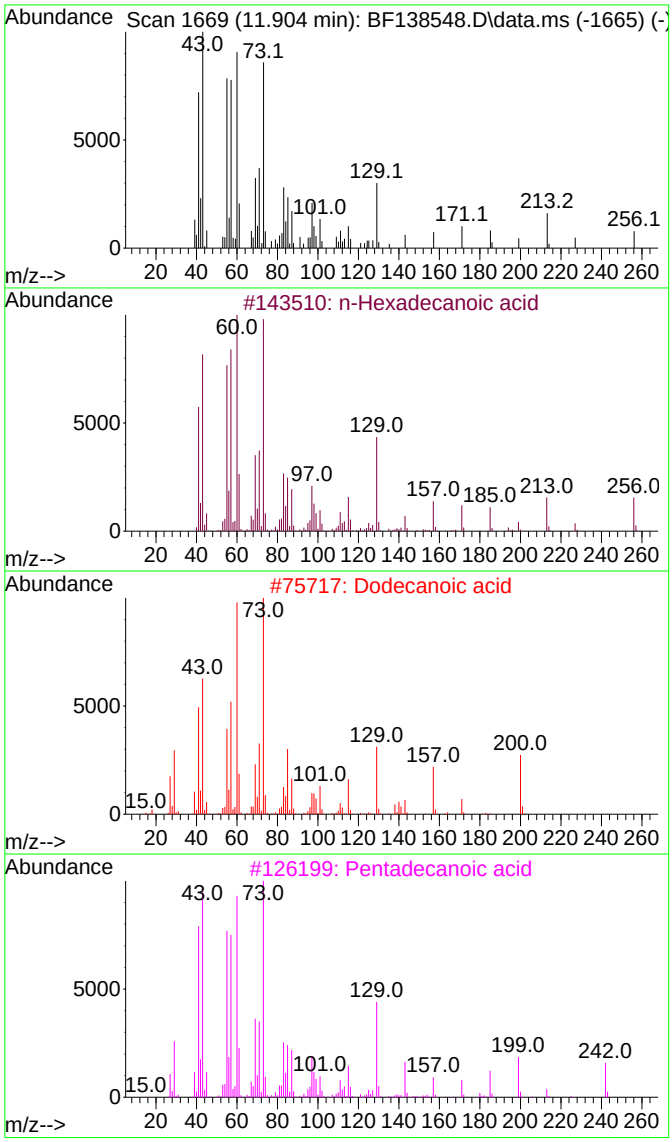
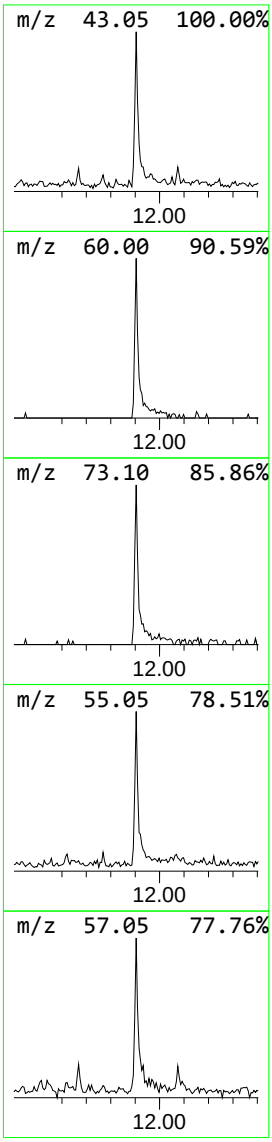
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	2.78 ng	93684	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Dodecanoic acid	200	C12H24O2	000143-07-7	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





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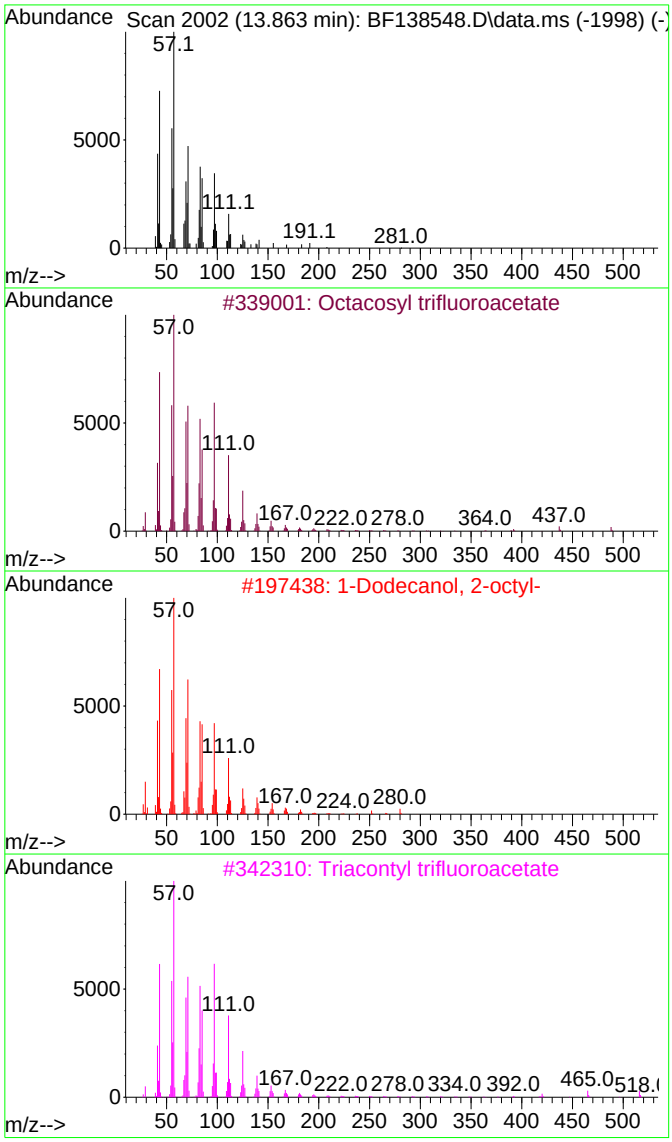
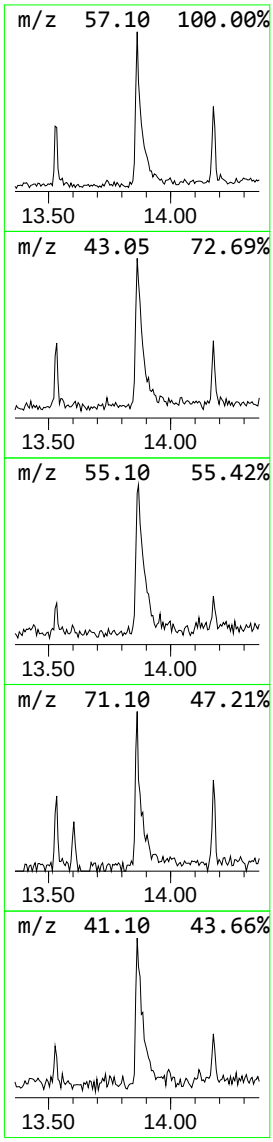
Peak Number 6 Octacosyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	6.36 ng	144276	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
3	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	90
4	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	90
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	90





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.169	73.3	ng	2033970	1	6.863	554944	20.0
unknown3.393	3.393	2.5	ng	68308	1	6.863	554944	20.0
2-Pentanone, 4-...	5.087	5.5	ng	154026	1	6.863	554944	20.0
1-Phenoxypropan...	8.451	2.5	ng	91626	2	8.145	730061	20.0
n-Hexadecanoic ...	11.904	2.8	ng	93684	4	11.380	674113	20.0
Octacosyl trifl...	13.863	6.4	ng	144276	5	14.015	453824	20.0