LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138844.D
Acq On : 07 Aug 2024 16:05
Operator : RC/JU
Sample : P3451-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
921-J-WS-080124

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138844.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	15	rVB	1461313	2268073	100.00%	22.214%
2	5.057	500	504	519	rVB	27474	39857	1.76%	0.390%
3	5.469	569	574	590	rBV	422082	558182	24.61%	5.467%
4	6.481	741	746	757	rBV	258075	352105	15.52%	3.449%
5	6.669	771	778	790	rBV	21270	35256	1.55%	0.345%
6	6.839	802	807	812	rBV	232106	287660	12.68%	2.817%
7	7.404	897	903	908	rBV	670544	908040	40.04%	8.894%
8	7.657	941	946	953	rBB	25747	32563	1.44%	0.319%
9	8.116	1019	1024	1030	rBV	293985	384558	16.96%	3.767%
10	8.434	1073	1078	1094	rBV	92417	135851	5.99%	1.331%
11	9.192	1201	1207	1212	rBV	1296191	1665432	73.43%	16.312%
12	9.869	1317	1322	1330	rBV	333359	420145	18.52%	4.115%
13	10.663	1452	1457	1467	rBV	681334	884572	39.00%	8.664%
14	11.357	1570	1575	1589	rBV	310840	388422	17.13%	3.804%
15	11.880	1659	1664	1680	rBV2	26781	54004	2.38%	0.529%
16	12.939	1838	1844	1849	rBV	925442	1179409	52.00%	11.552%
17	13.468	1928	1934	1942	rBV	22474	34274	1.51%	0.336%
18	13.845	1992	1998	2012	rBV2	23364	61035	2.69%	0.598%
19	13.998	2019	2024	2036	rVB	158676	211533	9.33%	2.072%
20	15.457	2266	2272	2285	rVB	147674	225499	9.94%	2.209%
21	16.327	2413	2420	2433	rBV8	26808	83445	3.68%	0.817%

Sum of corrected areas: 10209915

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Misc :
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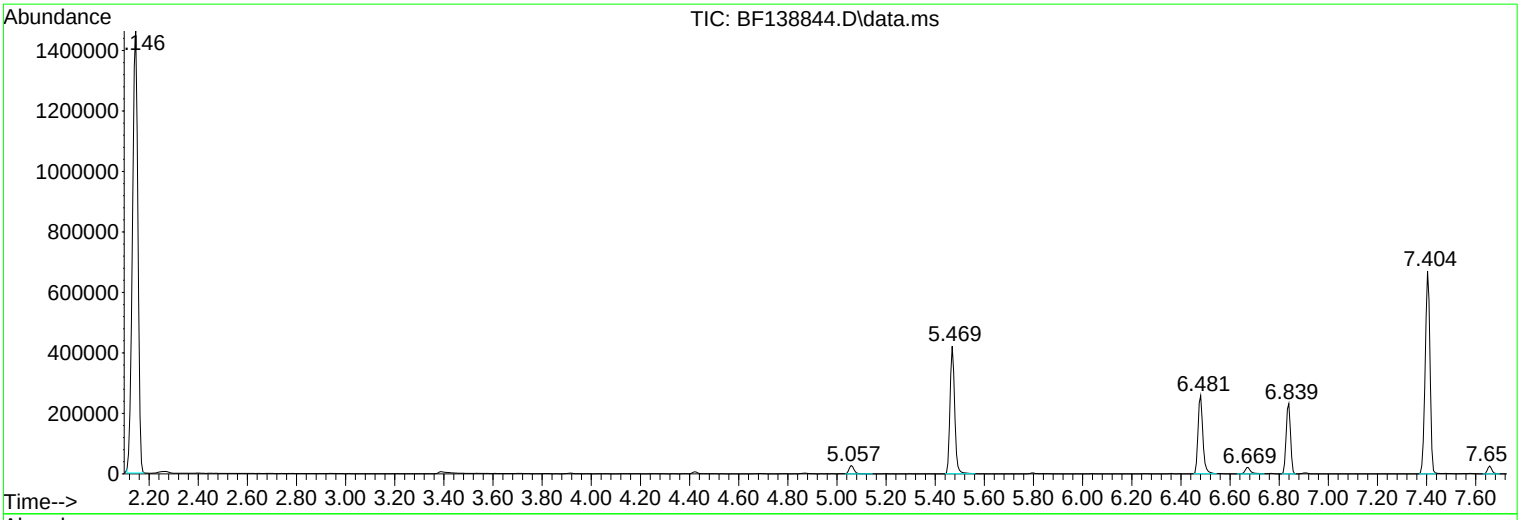
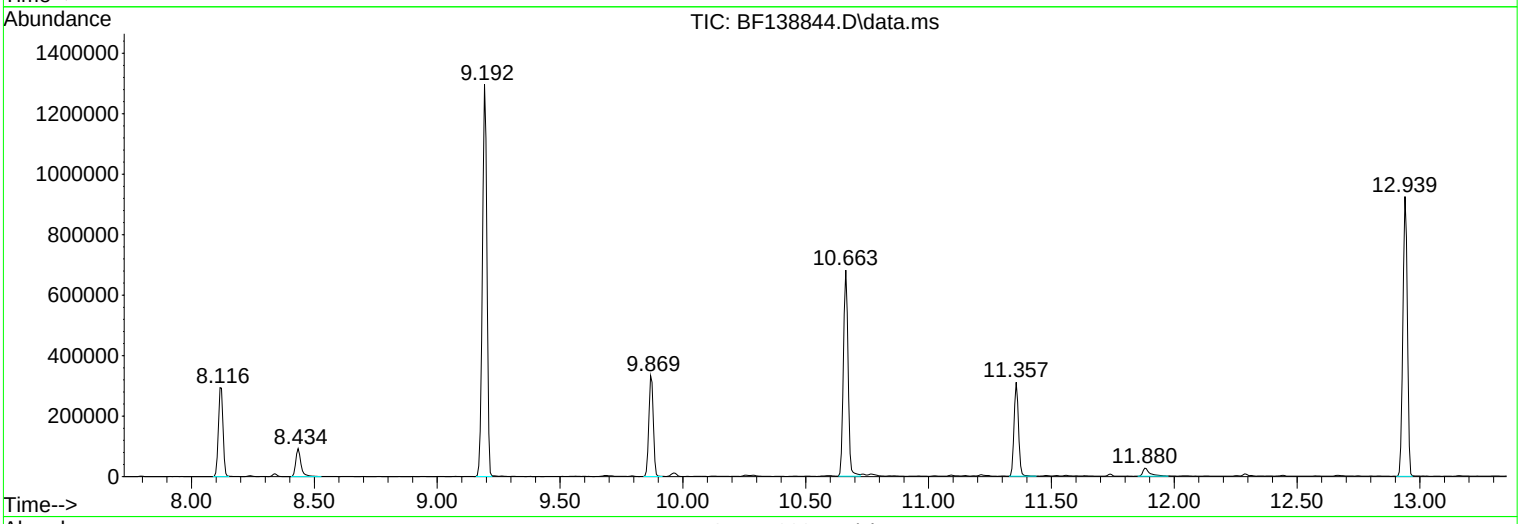
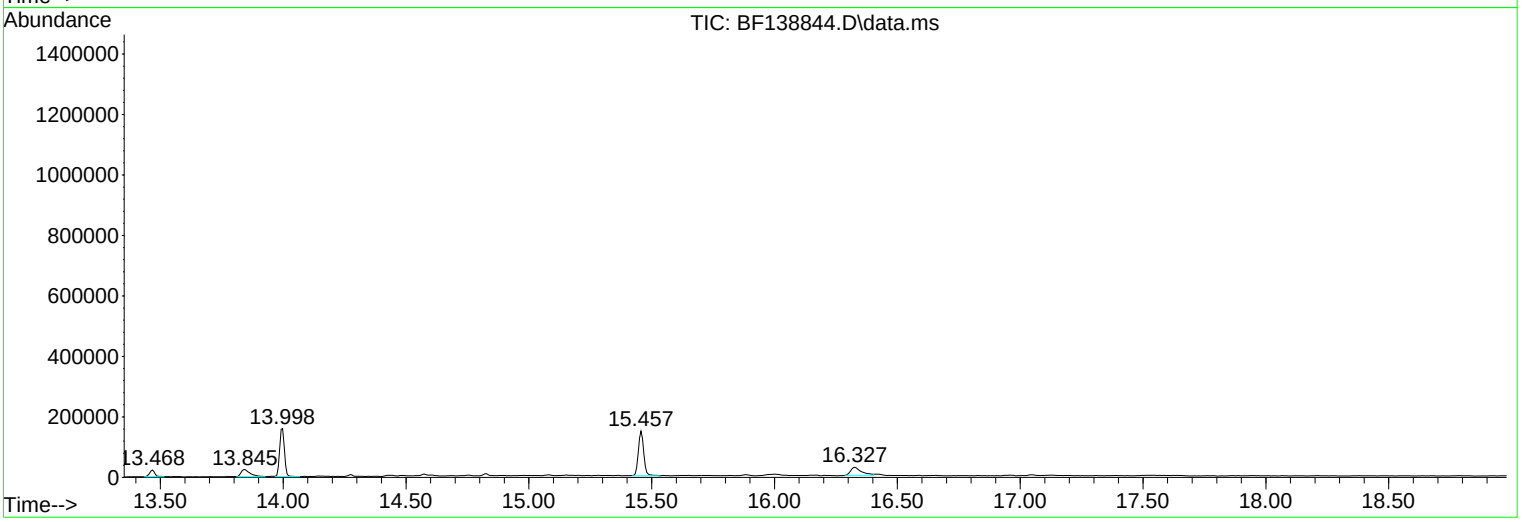
Instrument :
BNA_F
ClientSampleId :
921-J-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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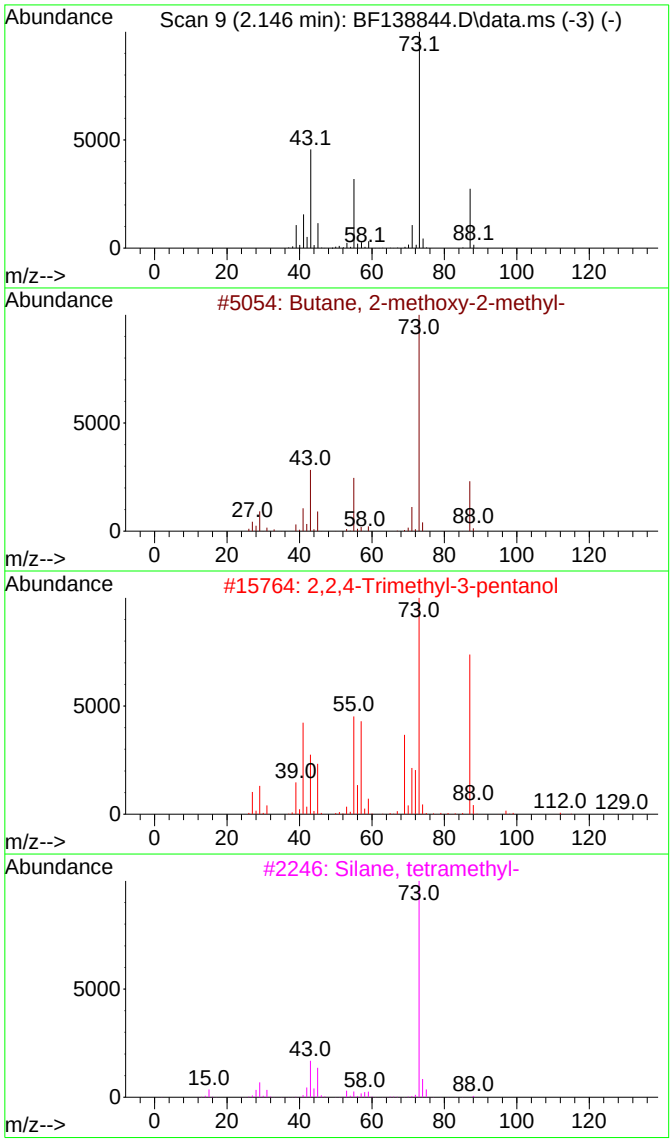
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

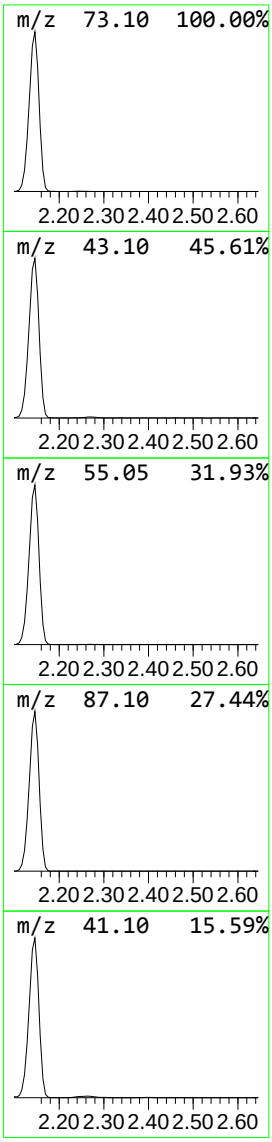
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	157.69 ng	2268070	1,4-Dichlorobenzene-d4	6.839

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	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Operator : RC/JU
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Instrument :
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ClientSampleId :
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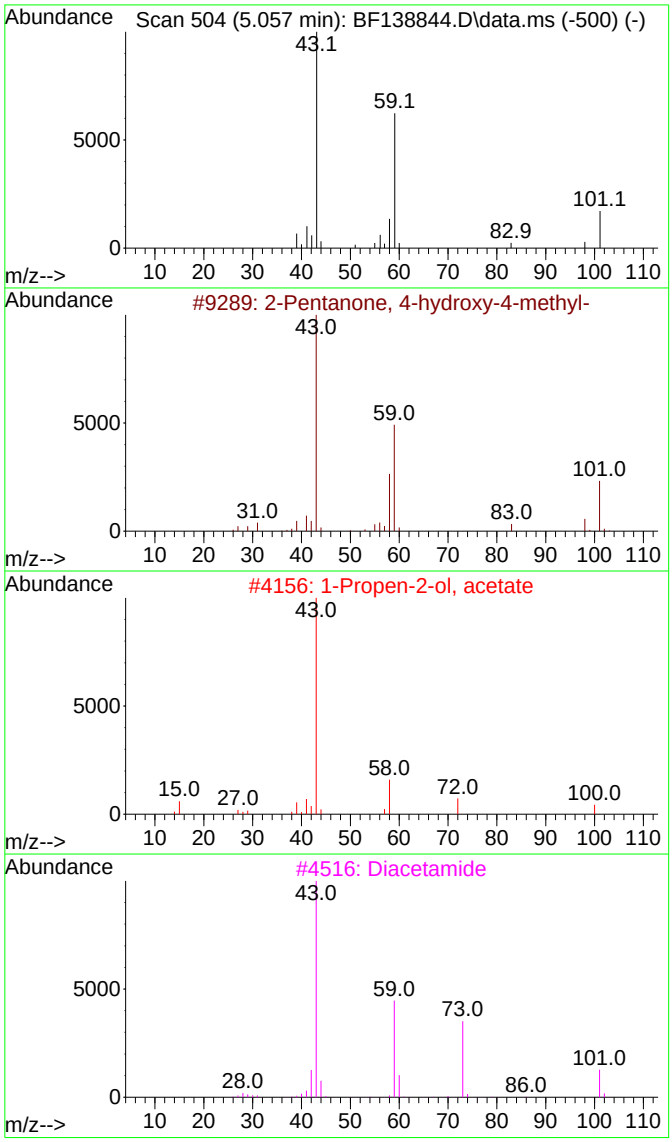
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

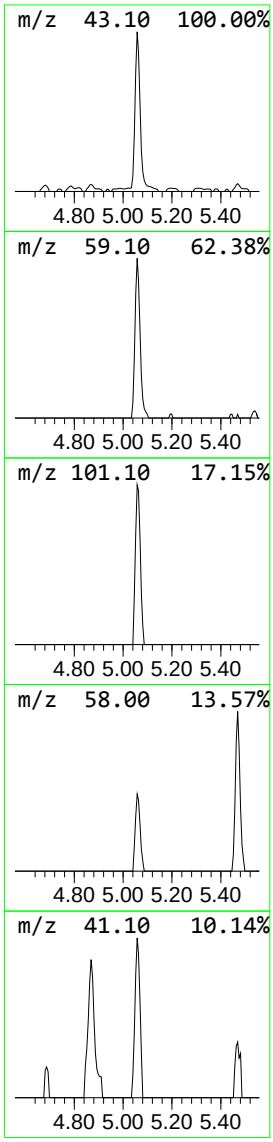
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	2.77 ng	39857	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





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Operator : RC/JU
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Misc :
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Instrument :
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ClientSampleId :
921-J-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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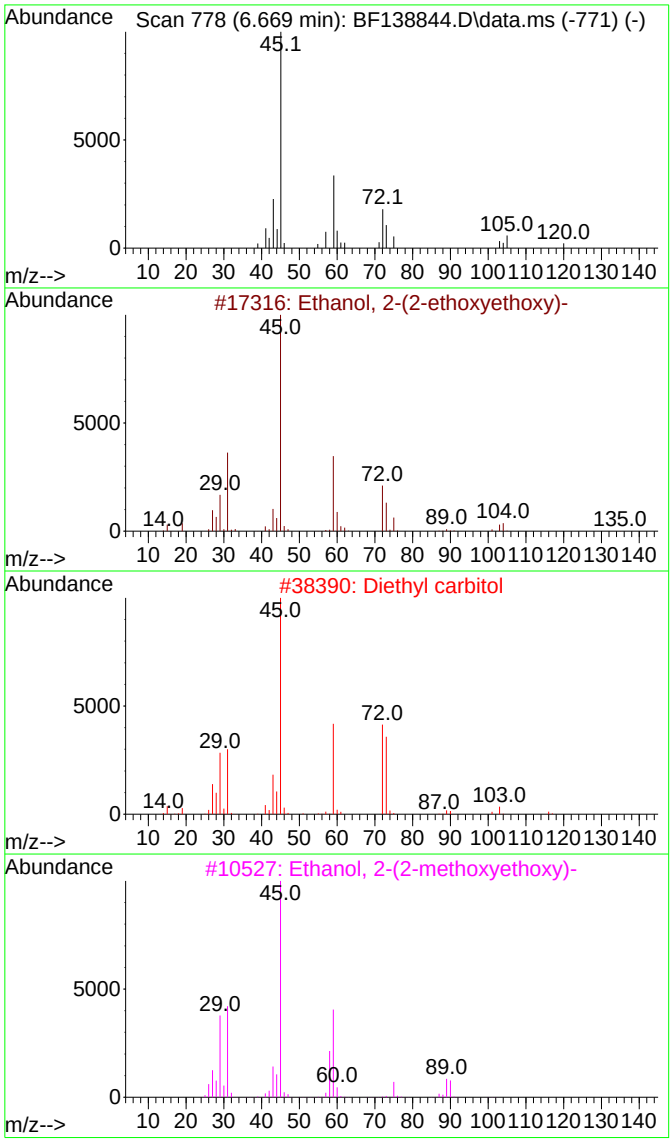
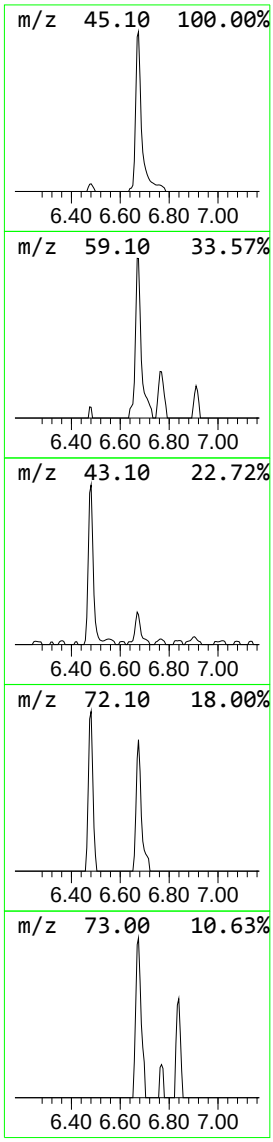
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.669	2.45 ng	35256	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	78
3	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
4	Hydrazinecarboxylic acid, ethyl ...	104	C3H8N2O2	004114-31-2	45
5	Ethyl ether	74	C4H10O	000060-29-7	42





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Instrument :
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ClientSampleId :
921-J-WS-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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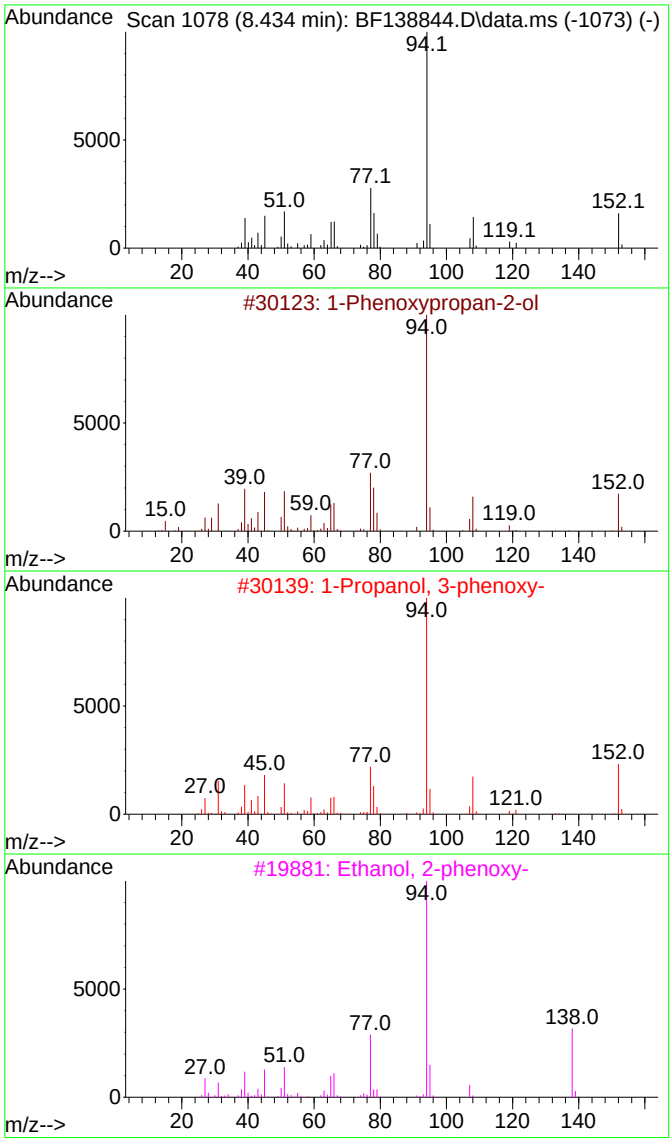
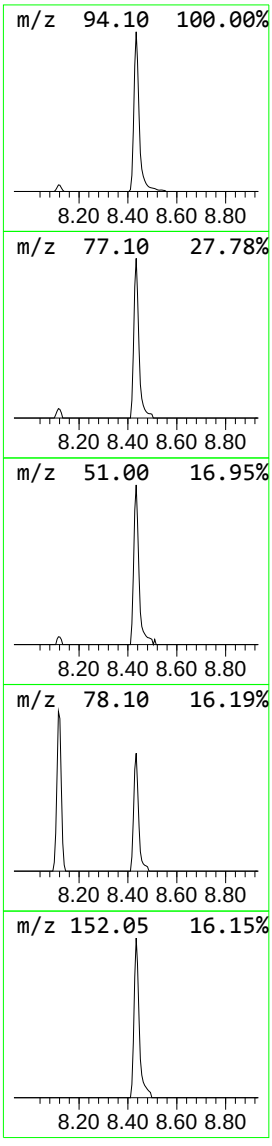
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.434	7.07 ng	135851	Naphthalene-d8	8.122

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	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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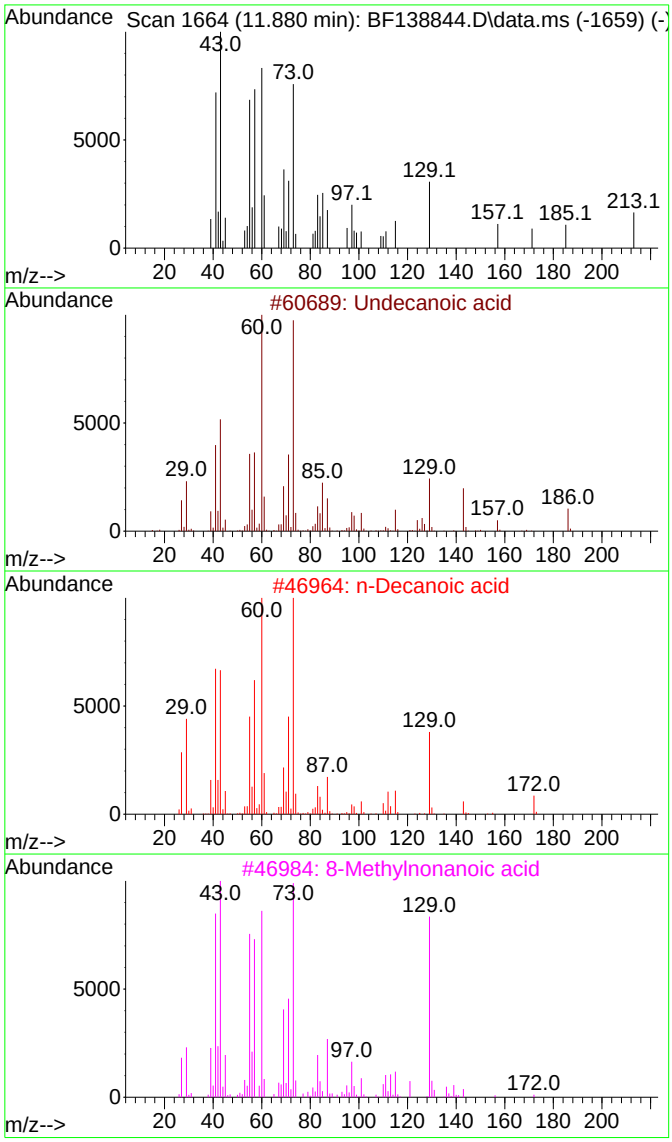
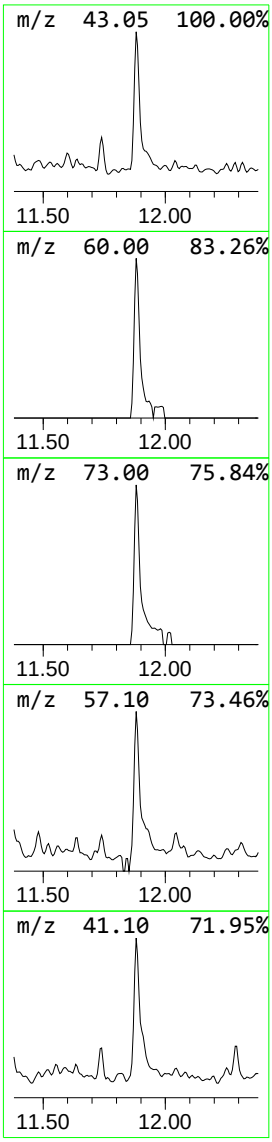
****

Peak Number 5 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	2.78 ng	54004	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	50
2	n-Decanoic acid	172	C10H20O2	000334-48-5	47
3	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	43
5	Melezitose	504	C18H32O16	000597-12-6	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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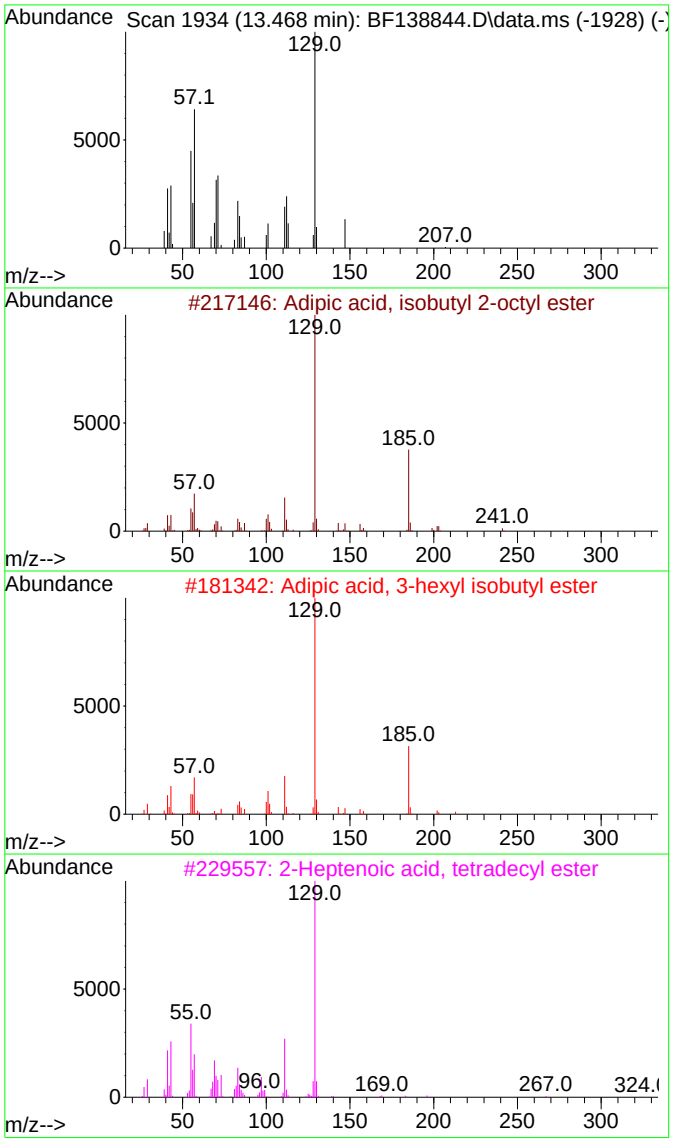
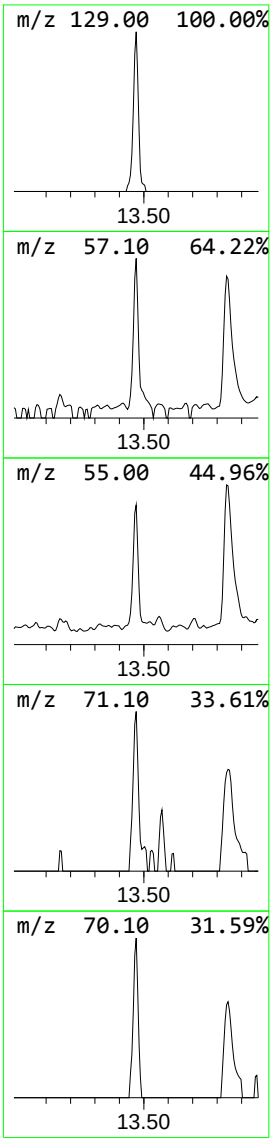
****
Peak Number 6 Adipic acid, isobutyl 2-oct... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.469	3.24 ng	34274	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	50
2	Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	47
3	2-Heptenoic acid, tetradecyl ester	324	C21H40O2	1000406-09-9	47
4	2-Heptenoic acid, dodecyl ester	296	C19H36O2	1000406-09-7	43
5	Adipic acid, isobutyl 3-pentyl e...	272	C15H28O4	1000324-60-4	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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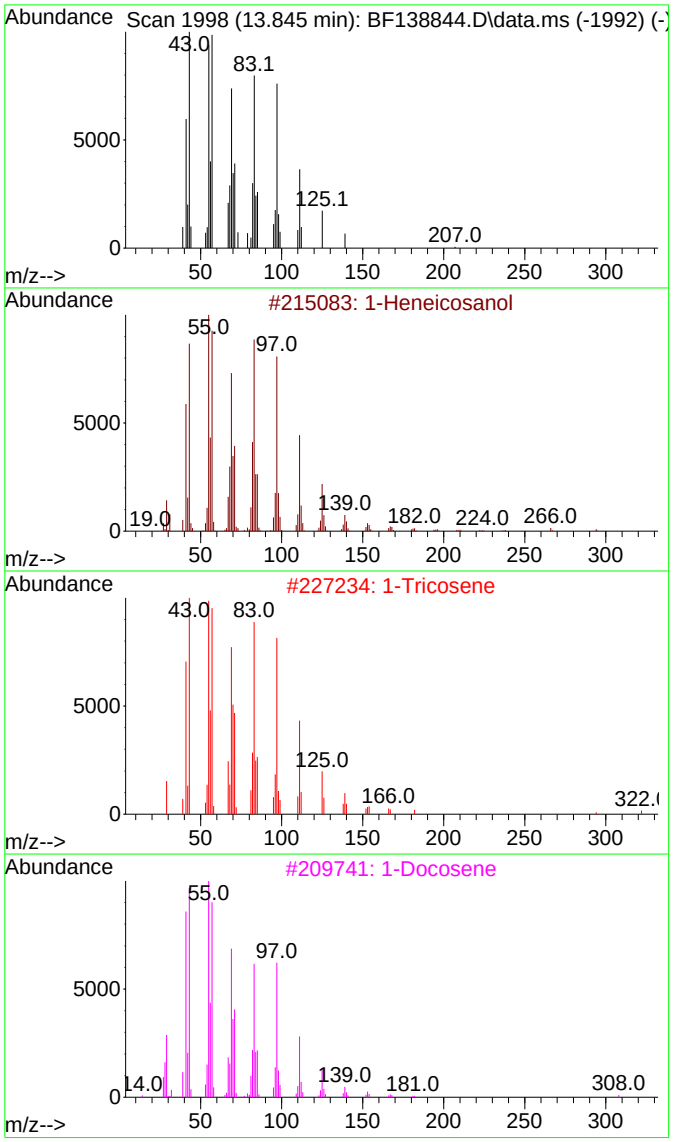
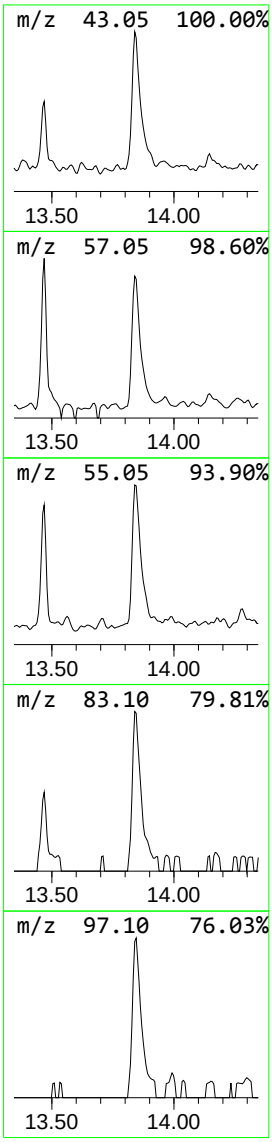
****

Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	5.77 ng	61035	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Tricosene	322	C23H46	018835-32-0	95
3	1-Docosene	308	C22H44	001599-67-3	93
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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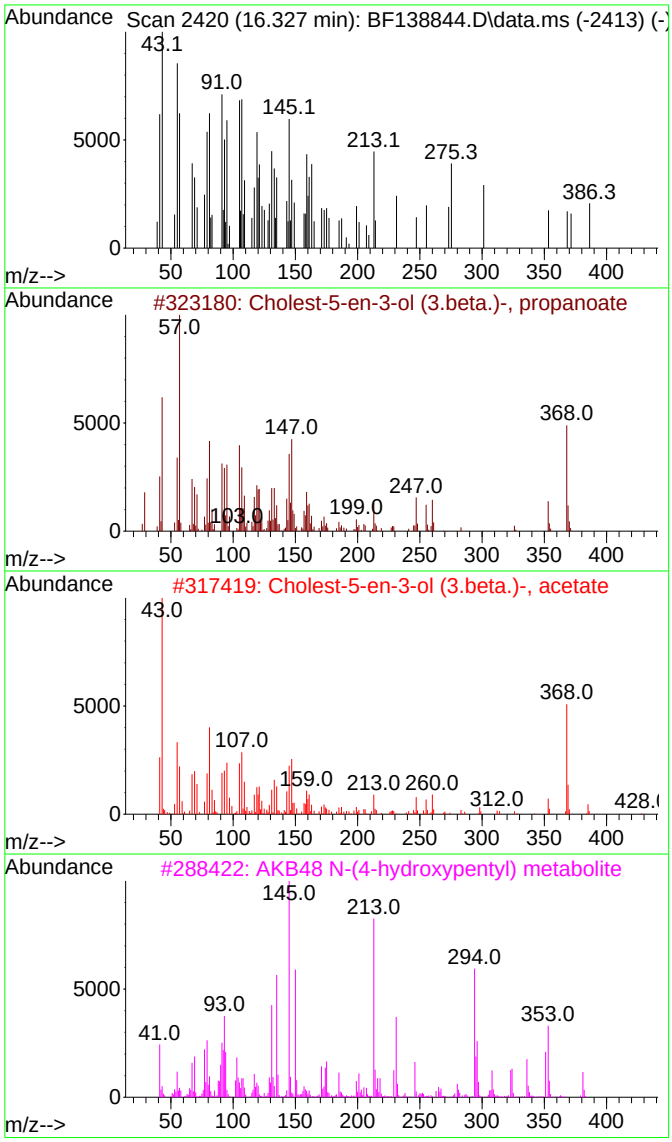
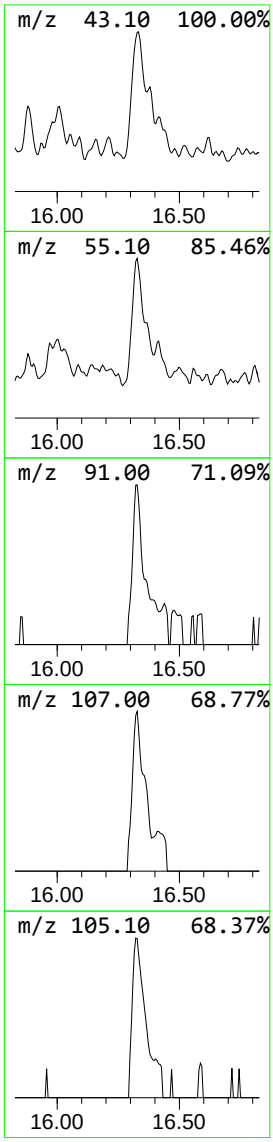
****

Peak Number 8 unknown16.327 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.327	7.40 ng	83445	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-en-3-ol (3.beta.)-, pr...	442	C30H50O2	000633-31-8	35
2	Cholest-5-en-3-ol (3.beta.)-, ac...	428	C29H48O2	000604-35-3	18
3	AKB48 N-(4-hydroxypentyl) metabo...	381	C23H31N3O2	1778734-77-2	14
4	cis-.alpha.-Copaene-8-ol	220	C15H24O	058569-25-8	14
5	Benzeneacetamide, .alpha.-ethyl-	163	C10H13NO	000090-26-6	11





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...	2.146	157.7	ng	2268070	1	6.839	287660	20.0
2-Pentanone, 4-...	5.057	2.8	ng	39857	1	6.839	287660	20.0
Ethanol, 2-(2-e...	6.669	2.5	ng	35256	1	6.839	287660	20.0
1-Phenoxypropan...	8.434	7.1	ng	135851	2	8.122	384558	20.0
Undecanoic acid	11.880	2.8	ng	54004	4	11.357	388422	20.0
Adipic acid, is...	13.469	3.2	ng	34274	5	13.998	211533	20.0
1-Heneicosanol	13.845	5.8	ng	61035	5	13.998	211533	20.0
unknown16.327	16.327	7.4	ng	83445	6	15.457	225499	20.0