LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110824\
Data File : BF140306.D
Acq On : 08 Nov 2024 18:29
Operator : RC/JU
Sample : P4756-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-B4

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-BF110524.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140306.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	4	11	23	rVB	1734322	2732573	94.58%	12.099%
2	2.269	24	30	40	rVB2	51072	87539	3.03%	0.388%
3	5.098	501	511	520	rBV	109305	173301	6.00%	0.767%
4	5.498	573	579	584	rBV	2029439	2637964	91.30%	11.681%
5	6.504	743	750	768	rBV	2017391	2791746	96.63%	12.361%
6	6.875	808	813	819	rVB	500875	646126	22.36%	2.861%
7	7.439	902	909	914	rBV	1293160	1696932	58.73%	7.514%
8	7.686	946	951	957	rBV	42952	55288	1.91%	0.245%
9	8.157	1021	1031	1039	rBV	620459	774645	26.81%	3.430%
10	8.369	1063	1067	1074	rVB	21022	30463	1.05%	0.135%
11	9.233	1208	1214	1219	rBV	2293518	2889191	100.00%	12.793%
12	9.916	1325	1330	1341	rVB	615084	768657	26.60%	3.404%
13	10.627	1446	1451	1459	rBV	269912	344591	11.93%	1.526%
14	10.704	1459	1464	1476	rBV	1205398	1627289	56.32%	7.205%
15	11.404	1578	1583	1591	rBV	575823	782648	27.09%	3.465%
16	11.933	1668	1673	1684	rBV	248369	388132	13.43%	1.719%
17	12.621	1787	1790	1795	rBV	37181	53442	1.85%	0.237%
18	12.721	1804	1807	1812	rBV	31682	48011	1.66%	0.213%
19	12.857	1827	1830	1839	rVB2	40725	72550	2.51%	0.321%
20	12.998	1848	1854	1859	rBV	2124237	2739790	94.83%	12.131%
21	13.892	2003	2006	2018	rVB2	131944	218945	7.58%	0.969%
22	14.057	2030	2034	2041	rVB	464293	605979	20.97%	2.683%
23	15.556	2285	2289	2298	rVB	264262	418433	14.48%	1.853%

Sum of corrected areas: 22584235

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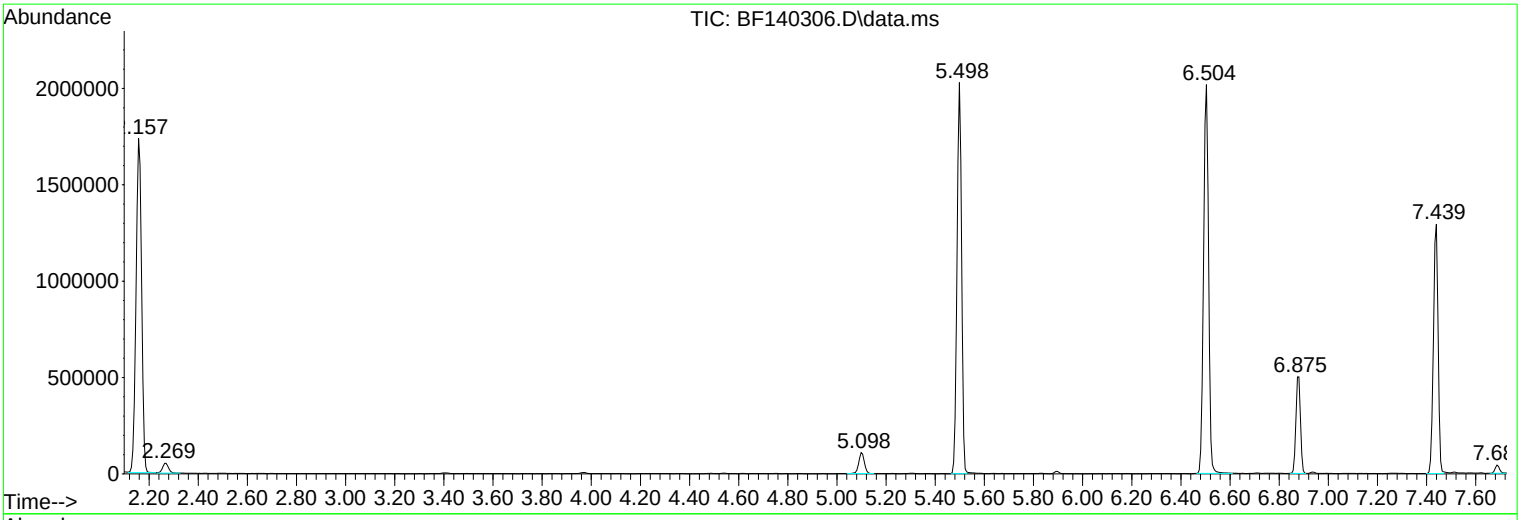
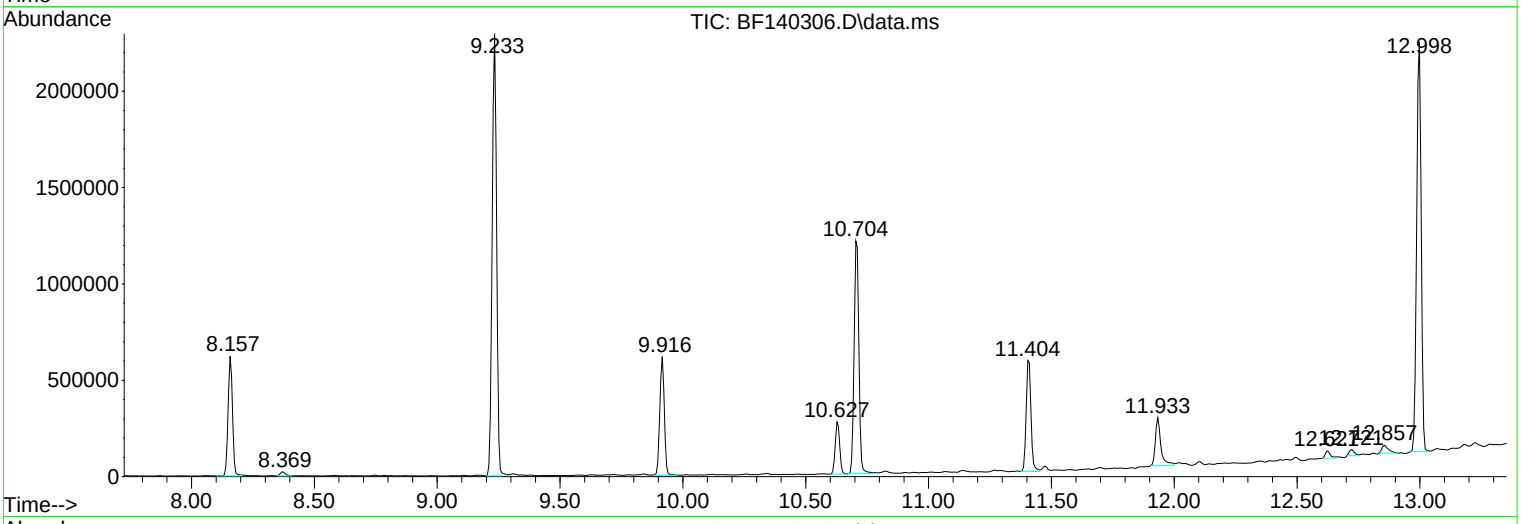
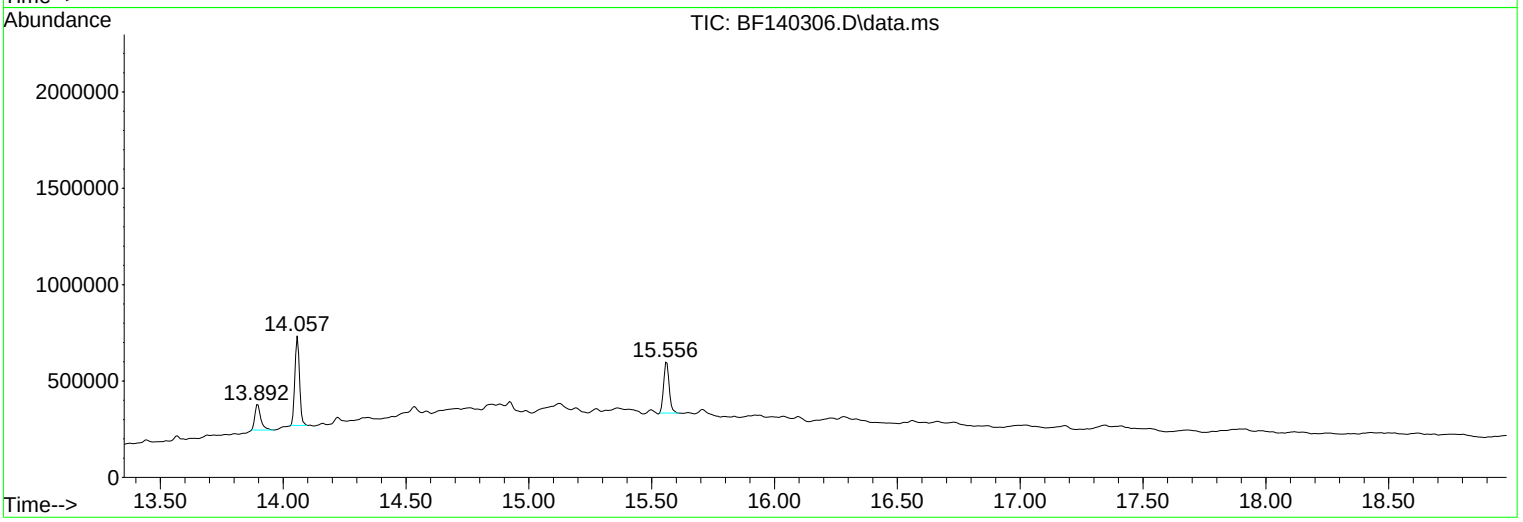
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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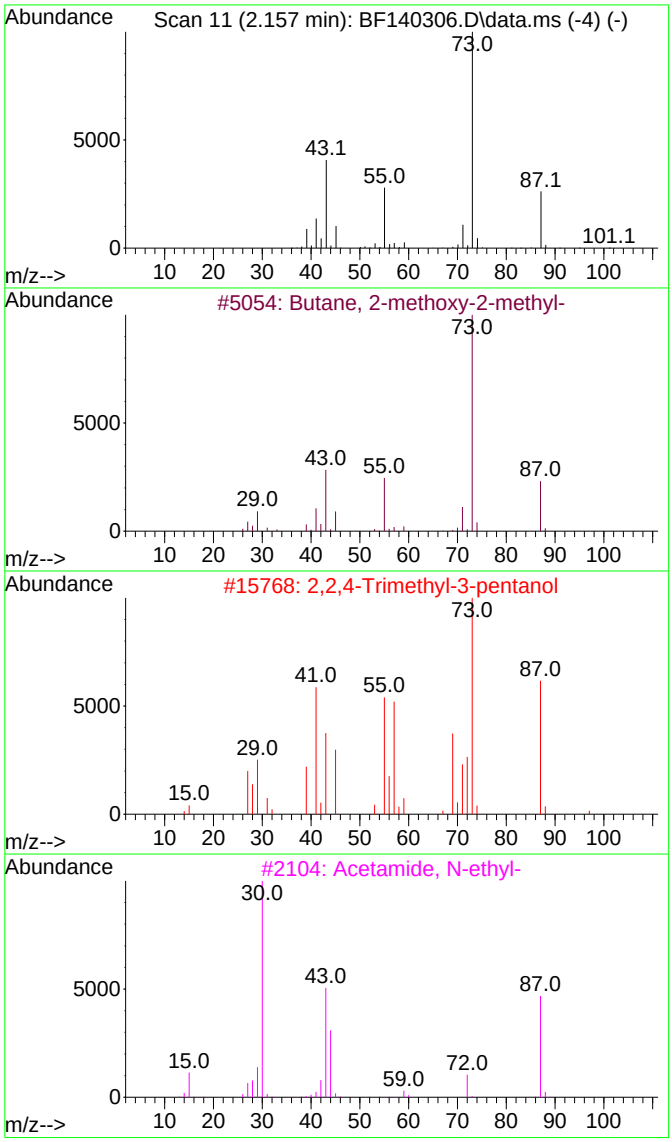
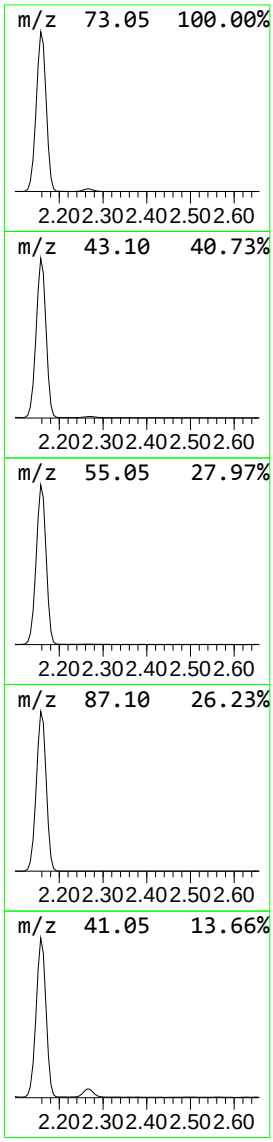
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	84.58 ng	2732570	1,4-Dichlorobenzene-d4	6.881

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	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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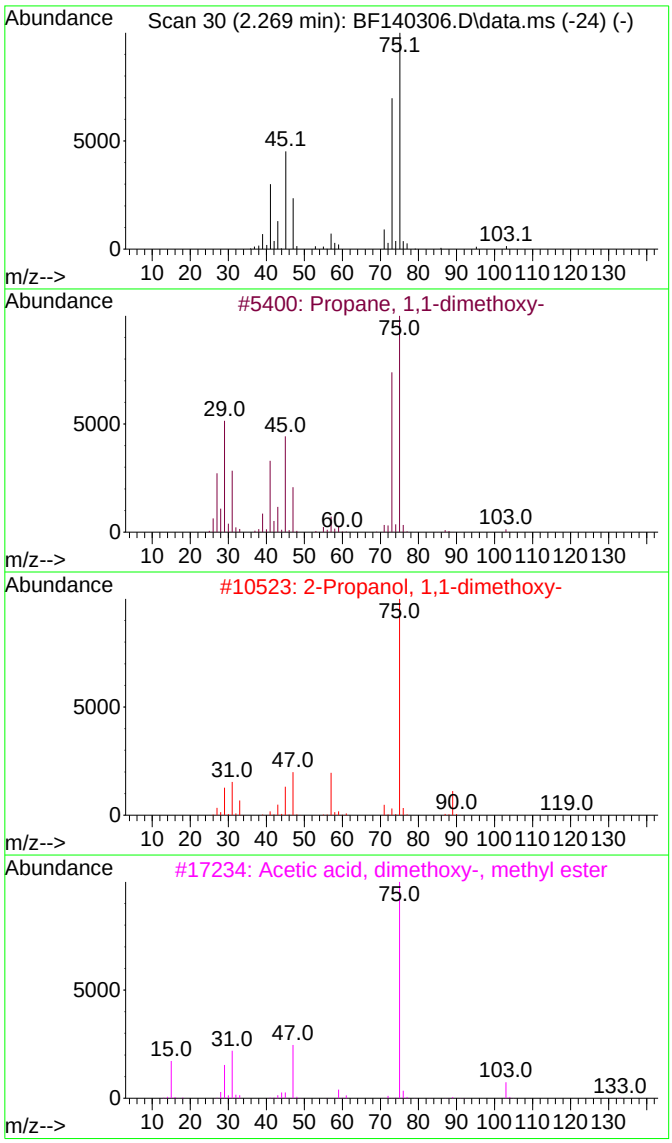
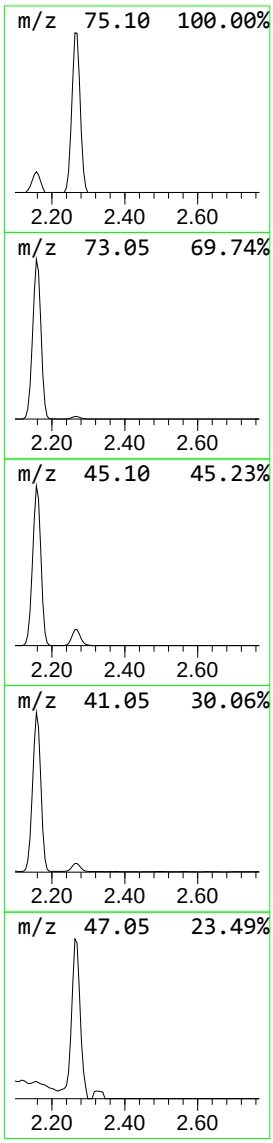
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	2.71 ng	87539	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	53
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	42
3	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	9
4	Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	9
5	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9





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Data File : BF140306.D
Acq On : 08 Nov 2024 18:29
Operator : RC/JU
Sample : P4756-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-B4

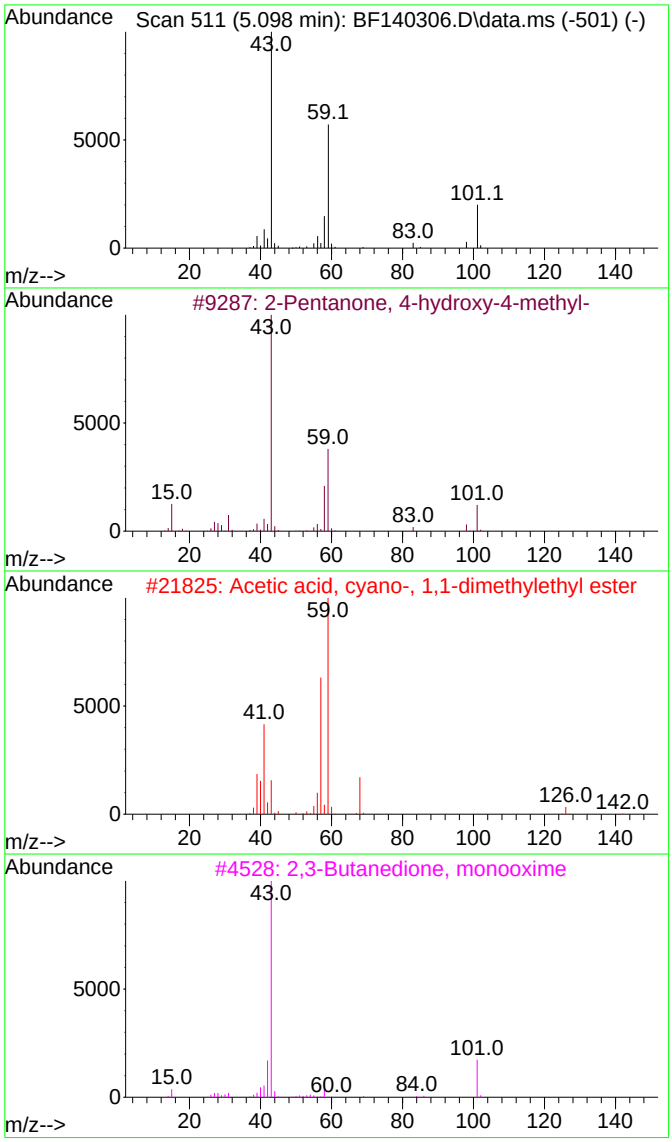
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

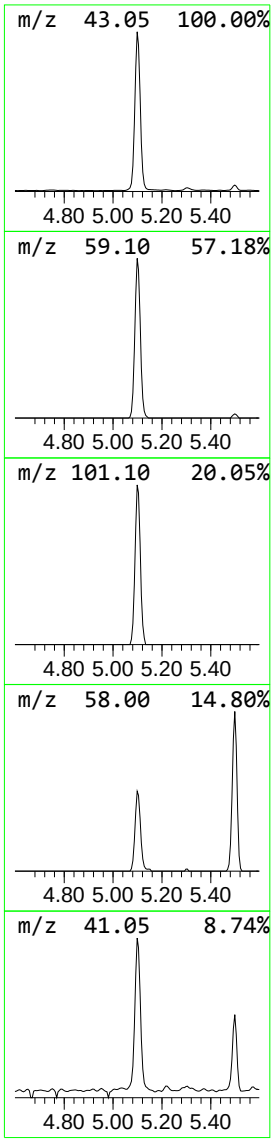
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	5.36 ng	173301	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Sample : P4756-01
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Instrument :
BNA_F
ClientSampleId :
BP-B4

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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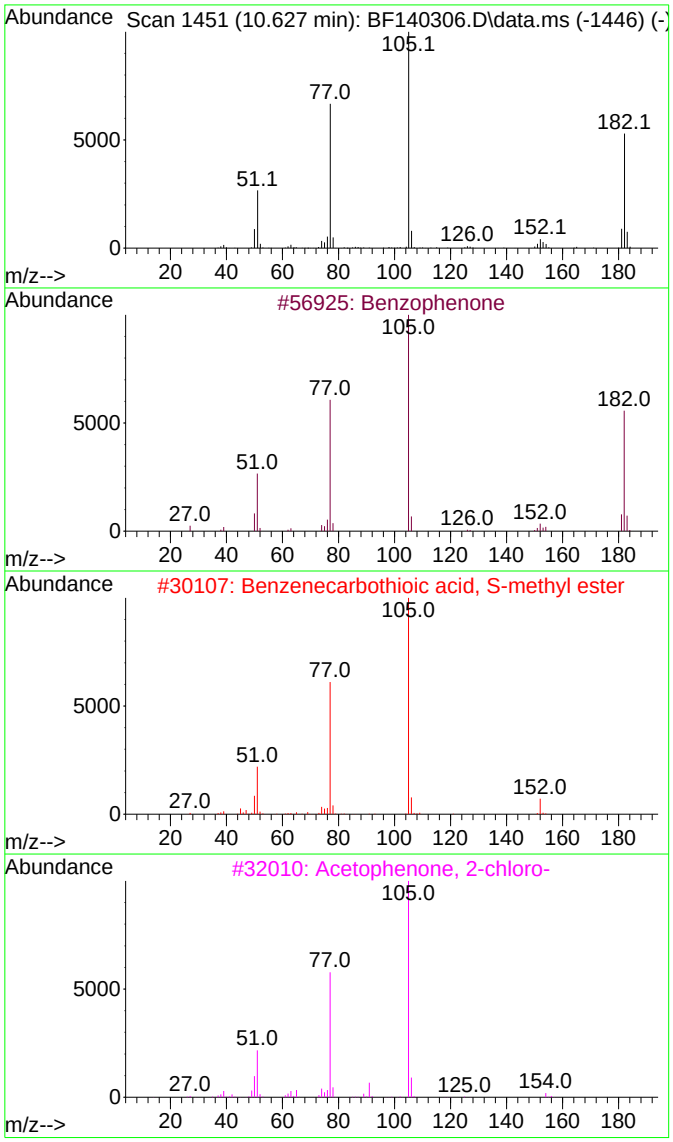
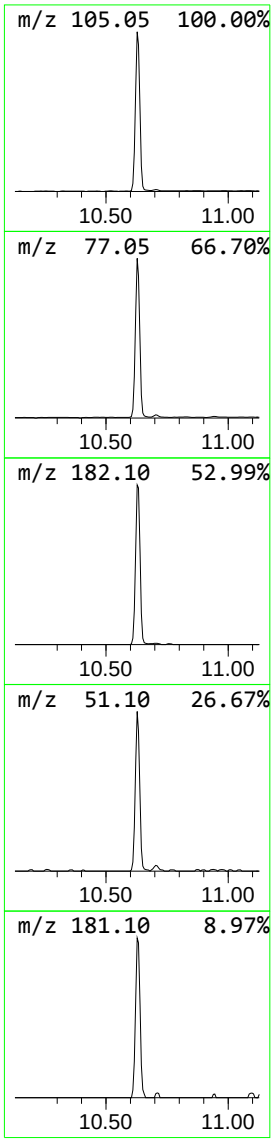
****

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.627	8.97 ng	344591	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





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BNA_F
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BP-B4

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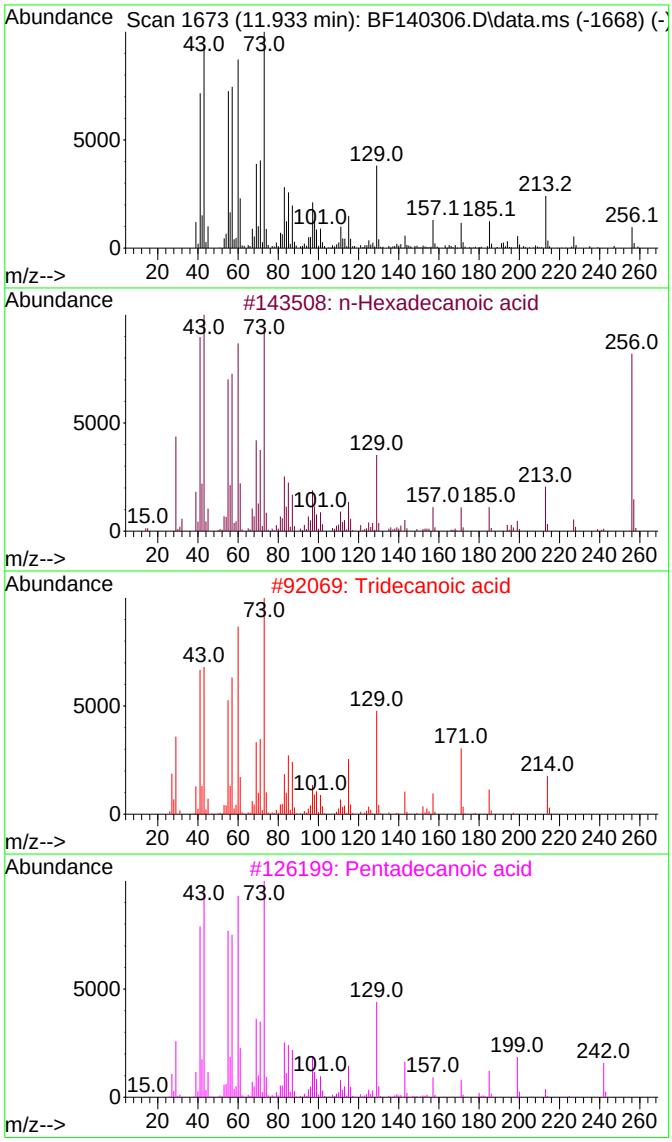
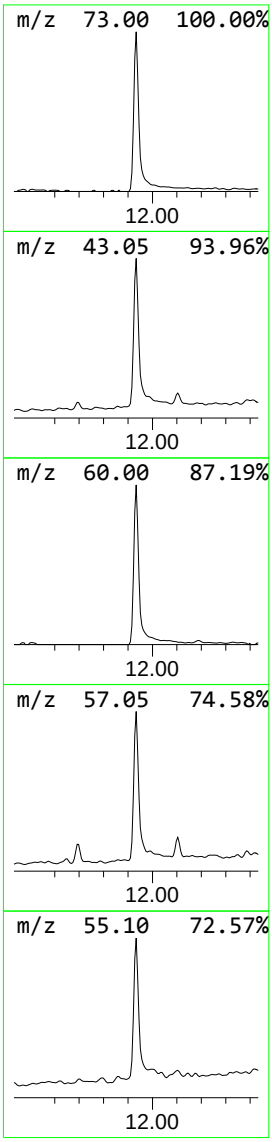
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	9.92 ng	388132	Phenanthrene-d10	11.404

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	Nonanoic acid	158	C9H18O2	000112-05-0	41





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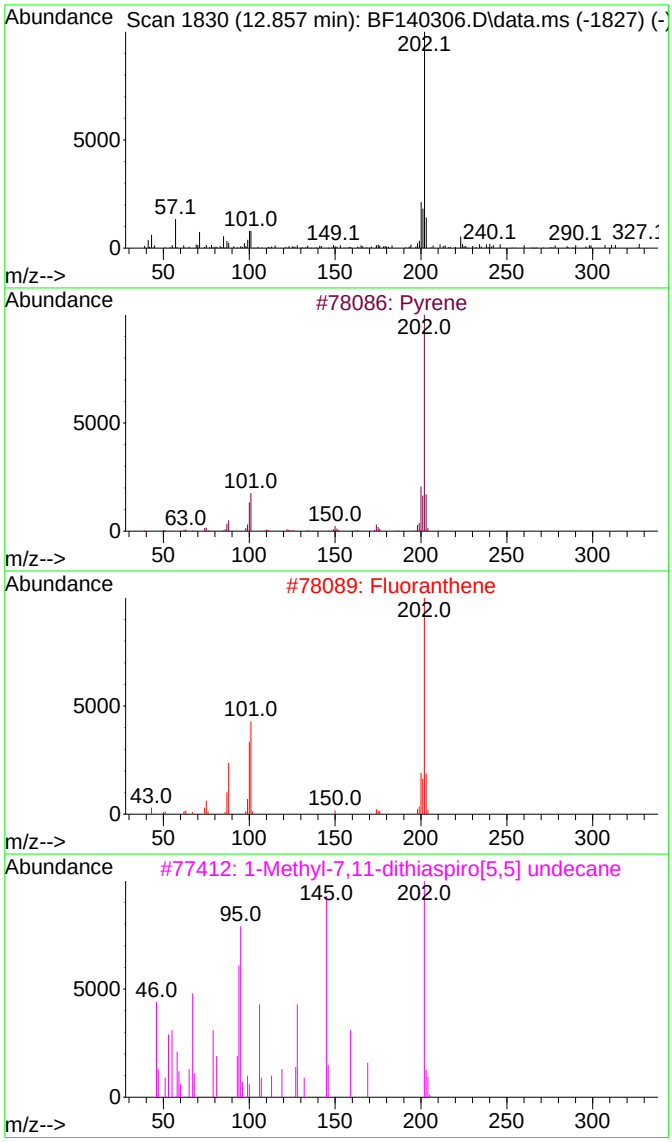
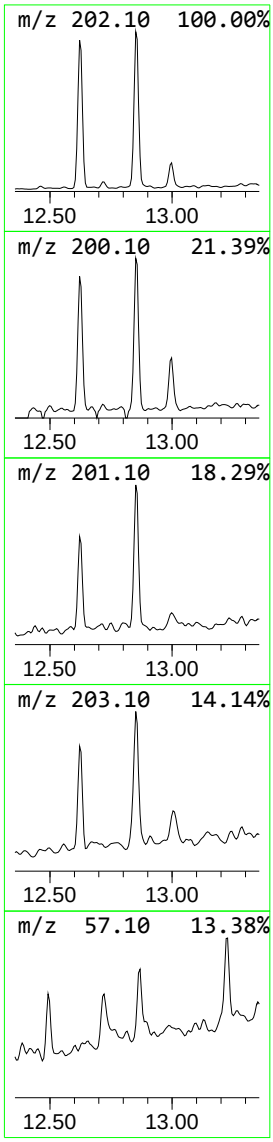
****

Peak Number 6 unknown12.857 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.857	2.39 ng	72550	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	76
2	Fluoranthene	202	C16H10	000206-44-0	68
3	1-Methyl-7,11-dithiaspiro[5,5] u...	202	C10H18S2	107678-22-8	47
4	6-Methyl -1-(trifluoromethyl)-3H...	202	C9H9F3N2	1000411-14-3	45
5	4,5-Dihydronaphtho(2,1-d)thiazol...	202	C11H10N2S	034176-49-3	45





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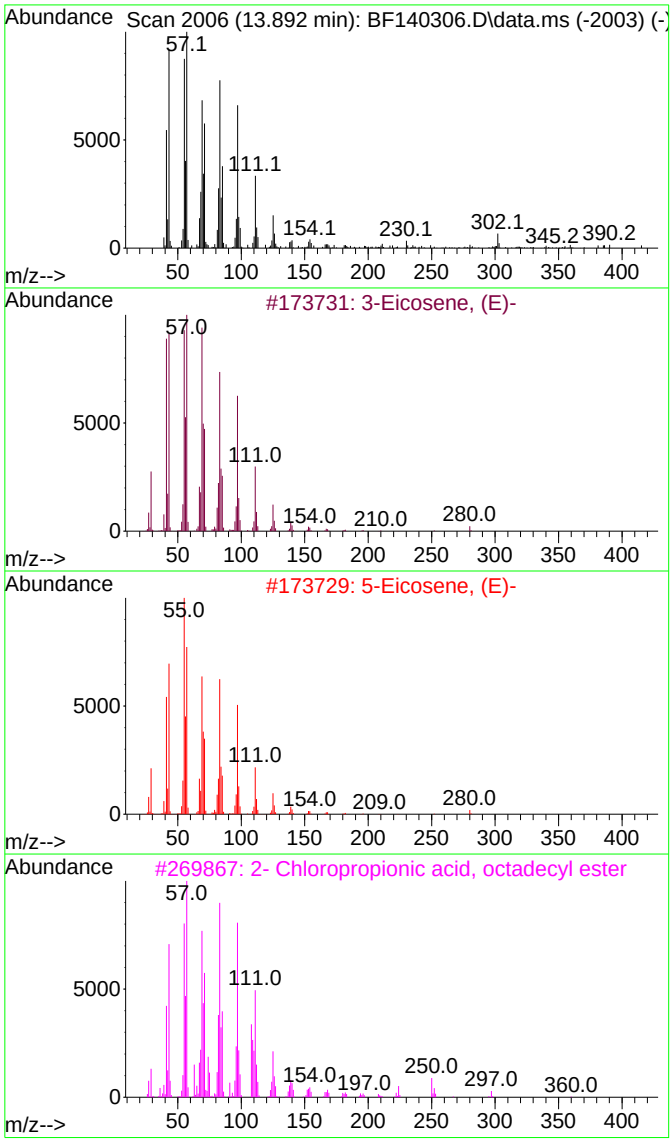
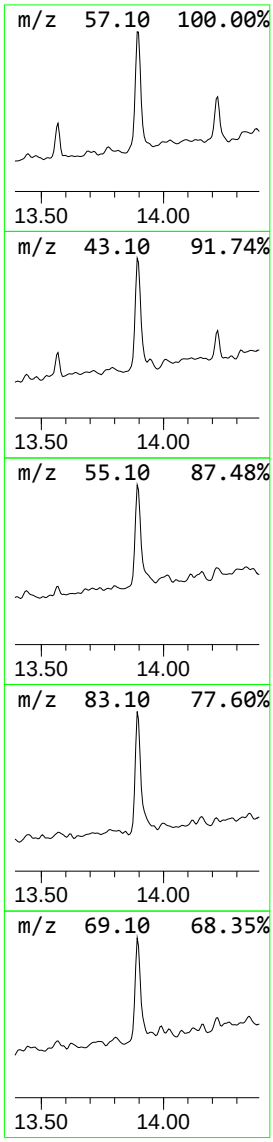
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	7.23 ng	218945	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	97
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





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...	2.157	84.6	ng	2732570	1	6.881	646126	20.0
Propane, 1,1-di...	2.269	2.7	ng	87539	1	6.881	646126	20.0
2-Pentanone, 4-...	5.098	5.4	ng	173301	1	6.881	646126	20.0
Benzophenone	10.627	9.0	ng	344591	3	9.916	768657	20.0
n-Hexadecanoic ...	11.933	9.9	ng	388132	4	11.404	782648	20.0
unknown12.857	12.857	2.4	ng	72550	5	14.057	605979	20.0
3-Eicosene, (E)-	13.892	7.2	ng	218945	5	14.057	605979	20.0