

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101023\
 Data File : BF135695.D
 Acq On : 10 Oct 2023 20:39
 Operator : CG\JU
 Sample : 04731-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DTP-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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135695.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.775	113	117	125	rBV2	28850	48457	2.19%	0.285%
2	4.334	379	382	392	rBV	191506	267139	12.06%	1.569%
3	4.969	484	490	506	rBV	1424396	1948620	87.97%	11.448%
4	5.381	556	560	575	rBV	1874656	2102873	94.93%	12.354%
5	5.763	622	625	630	rBV2	48734	49867	2.25%	0.293%
6	6.386	728	731	744	rBV	1922753	2091554	94.42%	12.287%
7	6.739	788	791	801	rVB	551769	483432	21.82%	2.840%
8	7.304	883	887	900	rBV	1432448	1326039	59.86%	7.790%
9	8.016	1005	1008	1015	rBV	701773	617099	27.86%	3.625%
10	9.092	1187	1191	1195	rBV	2294878	2215123	100.00%	13.013%
11	9.216	1208	1212	1221	rVB	342224	353805	15.97%	2.078%
12	9.774	1303	1307	1316	rBV	755222	656919	29.66%	3.859%
13	10.569	1438	1442	1456	rBV	1376873	1355005	61.17%	7.960%
14	11.269	1558	1561	1569	rBV	778503	668511	30.18%	3.927%
15	11.804	1649	1652	1663	rBV3	62320	86156	3.89%	0.506%
16	12.374	1744	1749	1752	rBV2	26412	26428	1.19%	0.155%
17	12.863	1828	1832	1836	rBV	2029845	1939669	87.56%	11.395%
18	13.933	2011	2014	2023	rVB	403598	397184	17.93%	2.333%
19	15.409	2260	2265	2273	rBV	265699	388295	17.53%	2.281%

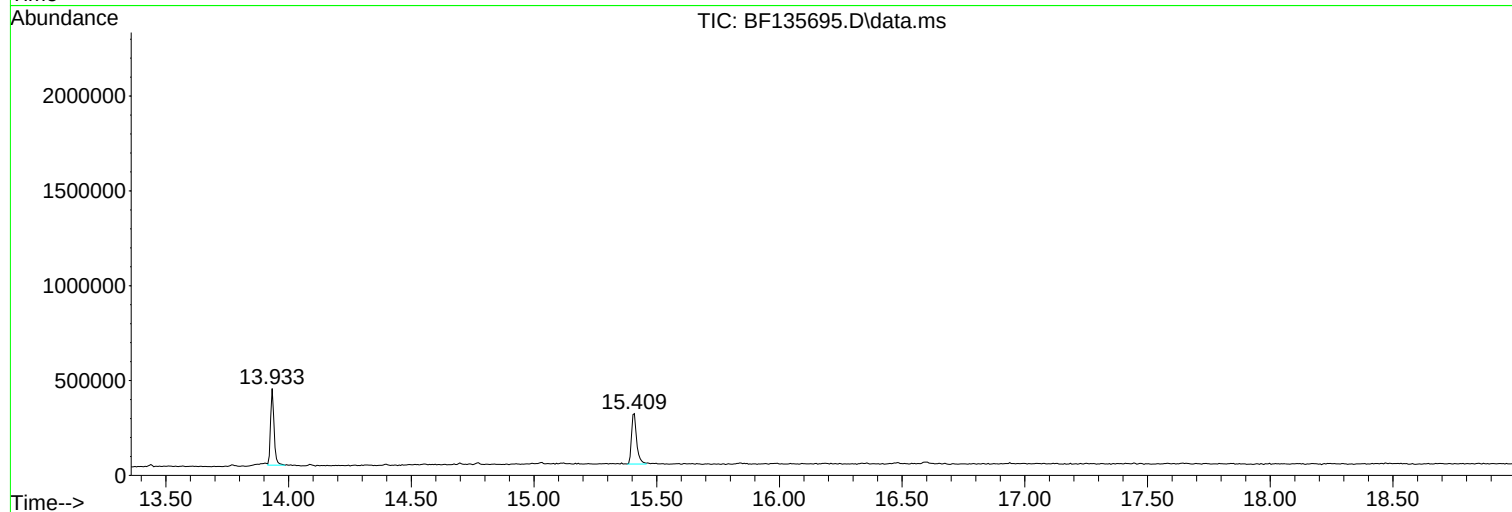
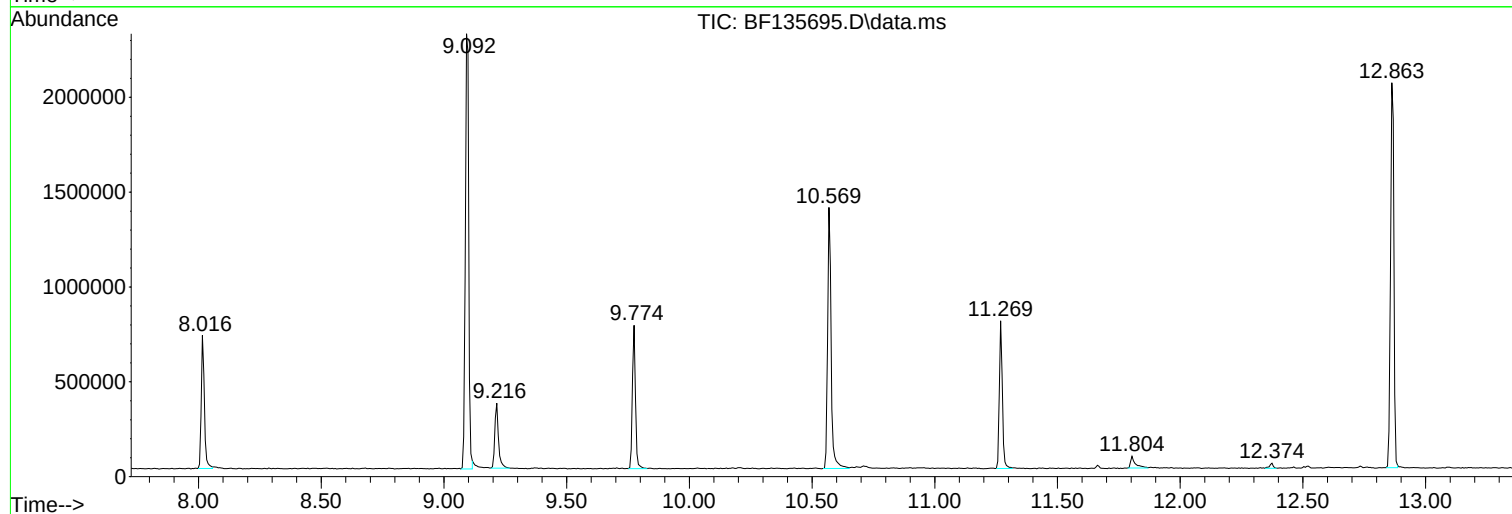
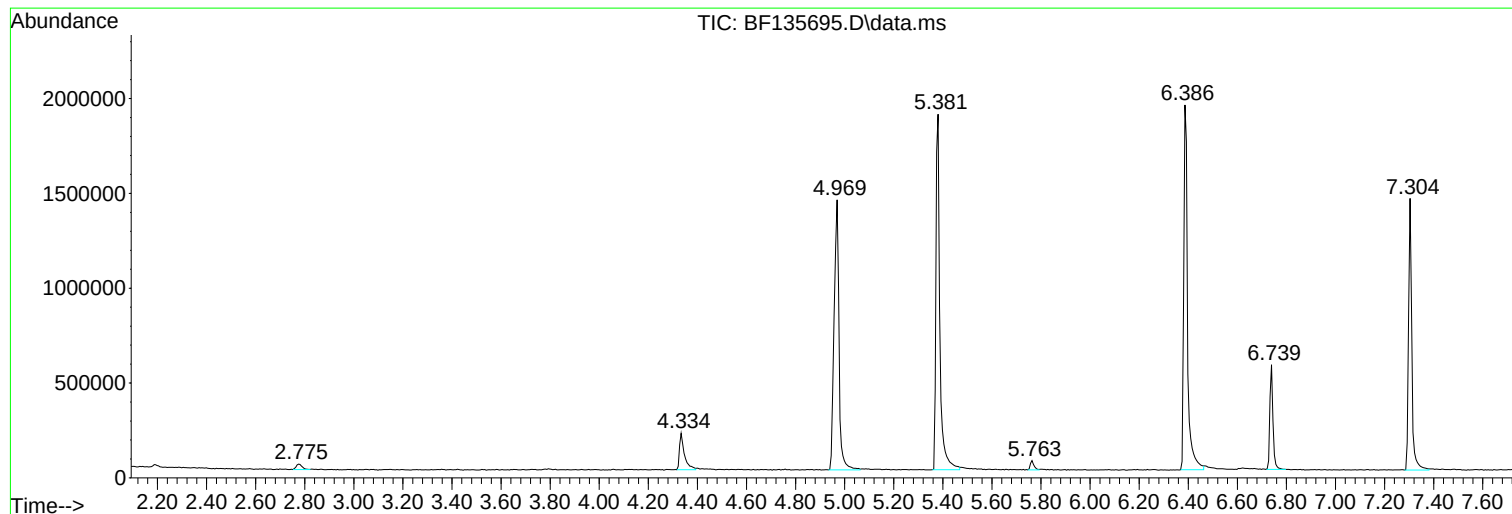
Sum of corrected areas: 17022175

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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\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.775	2.00 ng	48457	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	64
2			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	45
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	45
4			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	33
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	12

Peak Number 2 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.334	11.05 ng	267139	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4			2,4-Azetidinedione, 3,3-diethyl-	141	C7H11NO2	042282-85-9	78
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.969	80.62 ng	1948620	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.763	2.06 ng	49867	1,4-Dichlorobenzene-d4	6.739

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Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90		
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	37		
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17		
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10		
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10		

Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	10.77 ng	353805	Acenaphthene-d10	9.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87		
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53		
3	Metacetamol	151	C8H9NO2	000621-42-1	47		
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	47		
5	Acetaminophen	151	C8H9NO2	000103-90-2	47		

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	2.58 ng	86156	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94		
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86		
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80		
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80		
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	30		

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Dioxolane, ...	2.775	2.0	ng	48457	1	6.739	483432	20.0
3-Hexen-2-one	4.334	11.1	ng	267139	1	6.739	483432	20.0
2-Pentanone, 4-...	4.969	80.6	ng	1948620	1	6.739	483432	20.0
2-Pentanone, 4-...	5.763	2.1	ng	49867	1	6.739	483432	20.0
2,4,7,9-Tetrame...	9.216	10.8	ng	353805	3	9.774	656919	20.0
n-Hexadecanoic ...	11.804	2.6	ng	86156	4	11.269	668511	20.0