

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101023\
 Data File : BF135698.D
 Acq On : 10 Oct 2023 22:10
 Operator : CG\JU
 Sample : 04731-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DTP-1

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: BF135698.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.775	283	287	293	rVB3	17132	30046	1.49%	0.185%
2	4.340	380	383	393	rBV	43819	75435	3.74%	0.464%
3	4.963	484	489	501	rBV	1284522	1739496	86.34%	10.706%
4	5.375	556	559	581	rBV	1892886	2014670	100.00%	12.399%
5	5.763	620	625	630	rBV	41881	46263	2.30%	0.285%
6	6.386	728	731	744	rBV	1911045	1960198	97.30%	12.064%
7	6.598	765	767	783	rVB3	14722	38454	1.91%	0.237%
8	6.739	788	791	801	rVB	658688	587201	29.15%	3.614%
9	7.304	883	887	902	rBV	1390201	1265357	62.81%	7.788%
10	8.016	1005	1008	1022	rVB	829272	740513	36.76%	4.558%
11	9.092	1187	1191	1201	rBV	2203027	1996014	99.07%	12.285%
12	9.216	1208	1212	1217	rVB	31671	33183	1.65%	0.204%
13	9.774	1303	1307	1319	rVB	896681	772209	38.33%	4.753%
14	10.569	1439	1442	1455	rBV	1262269	1219595	60.54%	7.506%
15	11.269	1557	1561	1565	rBV	925161	781116	38.77%	4.807%
16	11.804	1649	1652	1664	rBV2	83145	110483	5.48%	0.680%
17	12.368	1743	1748	1755	rBV4	11257	23681	1.18%	0.146%
18	12.492	1765	1769	1774	rBV	50348	56624	2.81%	0.348%
19	12.727	1804	1809	1812	rBV	38744	43999	2.18%	0.271%
20	12.863	1828	1832	1836	rBV	1830373	1554579	77.16%	9.568%
21	13.439	1926	1930	1932	rBV2	25817	27266	1.35%	0.168%
22	13.768	1982	1986	1990	rBV2	24834	24058	1.19%	0.148%
23	13.868	1996	2003	2004	rBV6	16925	26320	1.31%	0.162%
24	13.933	2010	2014	2018	rBV	492574	455891	22.63%	2.806%
25	14.398	2089	2093	2096	rVB2	21854	24078	1.20%	0.148%
26	14.980	2190	2192	2196	rBV	17210	25774	1.28%	0.159%
27	15.404	2260	2264	2274	rBV	401579	528476	26.23%	3.253%
28	15.839	2335	2338	2343	rBV2	20110	22711	1.13%	0.140%
29	16.933	2520	2524	2531	rVB7	11834	24372	1.21%	0.150%

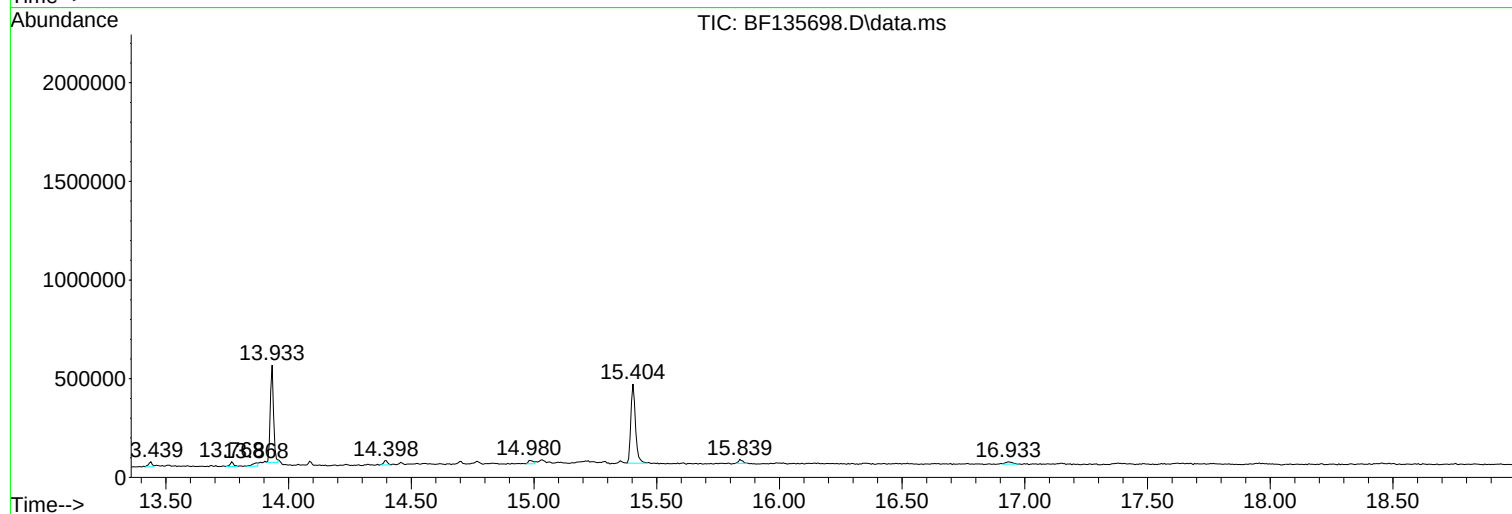
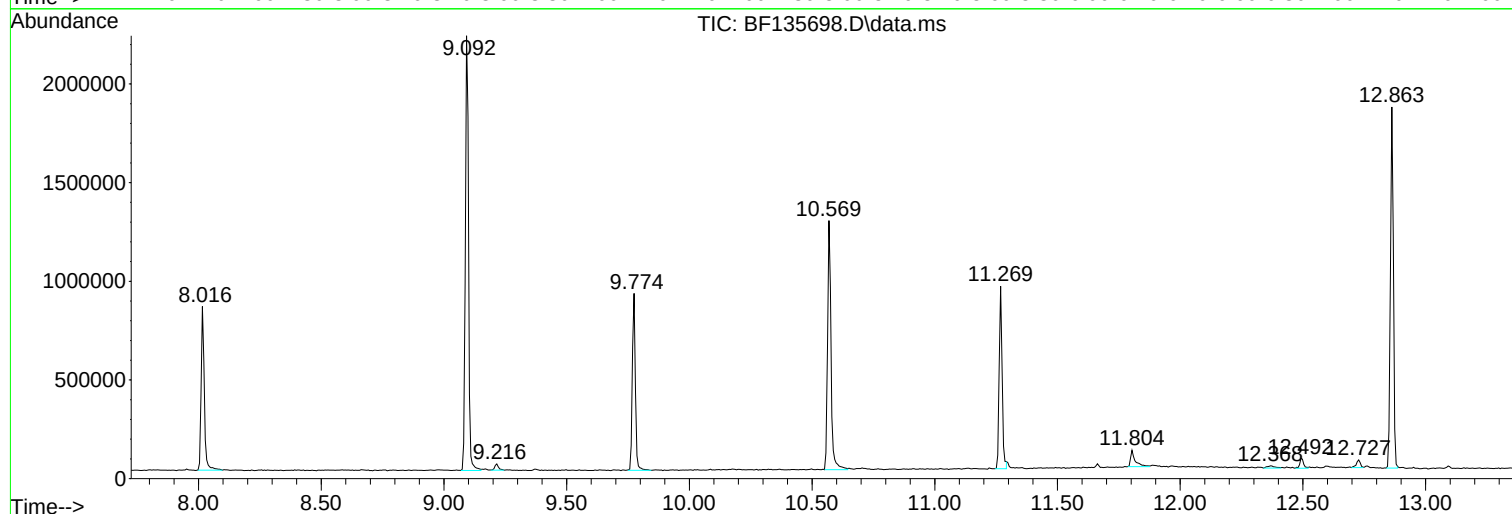
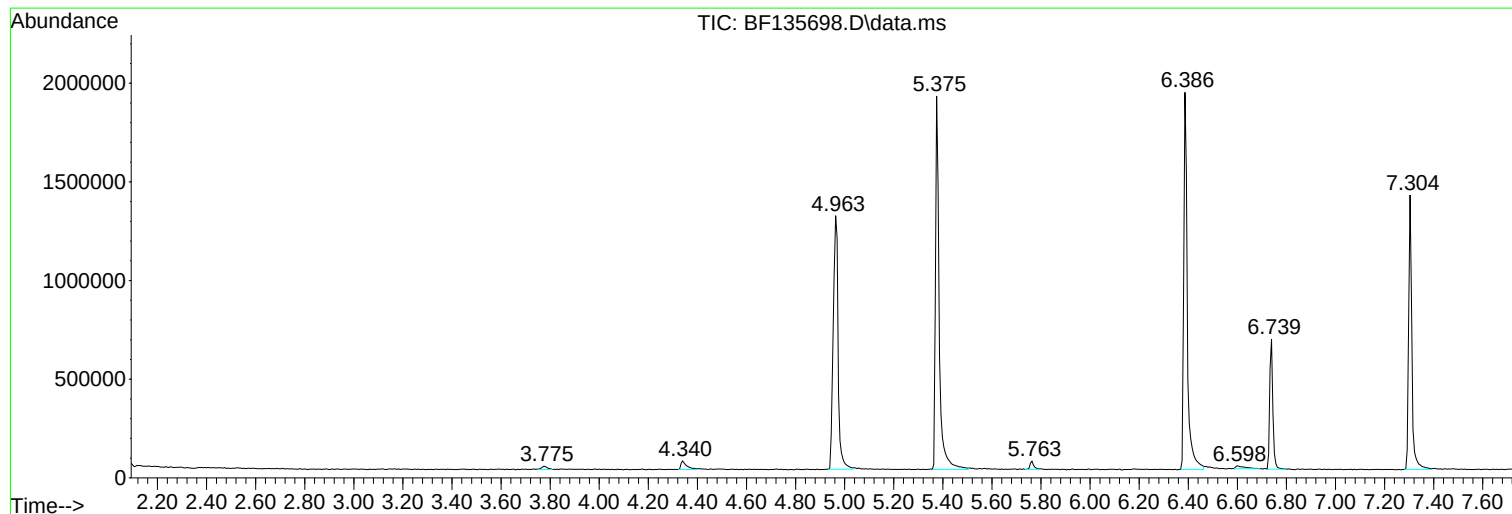
Sum of corrected areas: 16248062

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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 Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.340	2.57 ng	75435	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	90
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	83
3			Cyclohexane, methyl-	98	C7H14	000108-87-2	64
4			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	64
5			1H-Pyrazole, 4,5-dihydro-1,5-dim...	98	C5H10N2	005775-96-2	59

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	59.25 ng	1739500	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			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	2.83 ng	110483	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Dodecanoic acid	200	C12H24O2	000143-07-7	59
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	59

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.340	2.6	ng	75435	1	6.739	587201	20.0
2-Pentanone, 4-...	4.963	59.3	ng	1739500	1	6.739	587201	20.0
n-Hexadecanoic ...	11.804	2.8	ng	110483	4	11.269	781116	20.0