

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101319\
 Data File : BP000689.D
 Acq On : 13 Oct 2019 00:00
 Operator : JU
 Sample : K5348-12
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 1 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.958	481	488	491	rBV	2237178	2846723	49.27%	6.594%
2	5.369	555	558	576	rVB	936690	950296	16.45%	2.201%
3	6.387	727	731	742	rBV	3065533	2936093	50.82%	6.801%
4	6.516	750	753	757	rBV	2044564	1727205	29.89%	4.001%
5	6.746	789	792	796	rBV	1505863	1288571	22.30%	2.985%
6	6.816	801	804	811	rBV	87558	75894	1.31%	0.176%
7	6.905	815	819	822	rBV	4513924	3699539	64.03%	8.569%
8	7.310	883	888	891	rBV	3049861	2643488	45.75%	6.123%
9	7.528	921	925	928	rVB	94947	86556	1.50%	0.200%
10	8.034	1007	1011	1014	rBV	1859593	1609523	27.86%	3.728%
11	9.116	1191	1195	1198	rBV	6555012	5446914	94.27%	12.617%
12	9.510	1259	1262	1265	rBV	1049024	773604	13.39%	1.792%
13	9.793	1307	1310	1314	rVB	2092542	1896629	32.83%	4.393%
14	10.316	1396	1399	1402	rVB2	157697	140006	2.42%	0.324%
15	10.587	1442	1445	1453	rBV2	644320	656794	11.37%	1.521%
16	10.716	1464	1467	1475	rVB4	62714	108352	1.88%	0.251%
17	11.022	1516	1519	1521	rBV	70116	66272	1.15%	0.154%
18	11.157	1538	1542	1548	rBV	433651	417535	7.23%	0.967%
19	11.293	1561	1565	1568	rBV	2477954	2055343	35.57%	4.761%
20	11.316	1568	1569	1572	rVV	124750	69539	1.20%	0.161%
21	11.363	1574	1577	1581	rVB2	216003	194805	3.37%	0.451%
22	12.522	1770	1774	1777	rBV	305455	274231	4.75%	0.635%
23	12.751	1808	1813	1816	rBV	318906	305155	5.28%	0.707%
24	12.898	1834	1838	1842	rBV	6279585	5777687	100.00%	13.383%
25	13.087	1867	1870	1873	rVB	99833	97661	1.69%	0.226%
26	13.151	1878	1881	1884	rVB2	89163	91257	1.58%	0.211%
27	13.816	1990	1994	2001	rBV3	478666	657578	11.38%	1.523%
28	13.963	2014	2019	2022	rBV	2227122	2362550	40.89%	5.473%
29	13.992	2022	2024	2027	rVB	169157	141933	2.46%	0.329%
30	14.145	2047	2050	2054	rBV2	104341	94885	1.64%	0.220%
31	14.457	2100	2103	2106	rBV2	138103	130369	2.26%	0.302%
32	14.763	2152	2155	2158	rBV	101859	101051	1.75%	0.234%
33	15.016	2194	2198	2201	rBV	192319	296742	5.14%	0.687%
34	15.104	2210	2213	2220	rVB2	142979	209077	3.62%	0.484%

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Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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 >
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35	15.316	2246	2249	2255	rVB	146347	182677	3.16%	0.423%
36	15.375	2256	2259	2265	rBV	190397	253853	4.39%	0.588%
37	15.439	2266	2270	2275	rBV	1638153	1944451	33.65%	4.504%
38	15.928	2349	2353	2357	rBV	83734	126875	2.20%	0.294%
39	16.145	2388	2390	2404	rVB7	76204	168746	2.92%	0.391%
40	16.904	2515	2519	2525	rVB2	69685	123808	2.14%	0.287%
41	17.339	2589	2593	2604	rVB	65907	141042	2.44%	0.327%

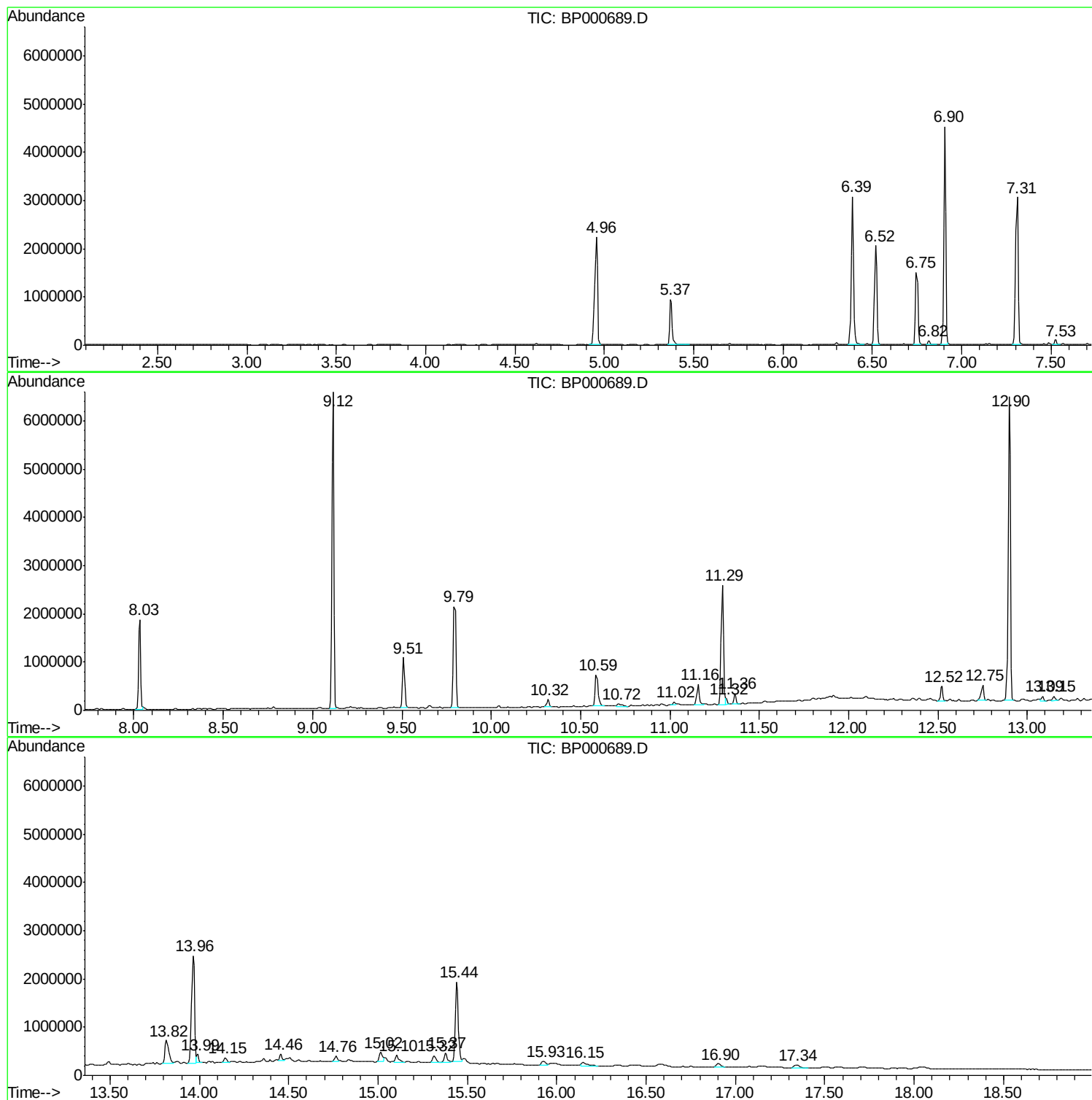
Sum of corrected areas: 43171309

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
4.96	44.18 ng	2846720	1,4-Dichlorobenzene-d4	6.75		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	45
2	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2		016504-58-8	43
3	Guanidine	59	CH5N3		000113-00-8	38
4	Acetone	58	C3H6O		000067-64-1	12
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	12

Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
6.52	26.81 ng	1727210	1,4-Dichlorobenzene-d4	6.75		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38	
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17	
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12	
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9	

Peak Number 3 1,2-Dichlorobenzene-D4 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
6.90	57.42 ng	3699540	1,4-Dichlorobenzene-d4	6.75		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	94
2		1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	94
3		Benzenamine, N,N-dimethyl-4-nitr...	150	C8H10N2O	000138-89-6	32
4		2-Bromo-2'-nitroacetophenone	243	C8H6BrNO3	006851-99-6	17
5		2,3,5-Tri-O-p-nitrobenzoyl-.alph...	606	C27H18N4O13	1000129-91-5	16

Peak Number 4 5,5,8a-Trimethyldecalin-1-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
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11.16	4.06 ng	417535	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5,8a-Trimethyldecalin-1-one	194	C13H22O	1000195-96-1	38
2	1-Methyl-3-n-propyl-2-pyrazolin-...	140	C7H12N2O	031272-04-5	27
3	Cyclohexanone, 3-(4-hydroxybutyl...	184	C11H20O2	091212-98-5	27
4	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	22
5	Phosphonic acid, methyl-, 2,2-di...	220	C10H21O3P	1000273-45-9	22

 Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.82	5.57 ng	657578	Chrysene-d12		13.96
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	97
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94

 Peak Number 6 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
15.10	2.15 ng	209077	Perylene-d12		15.44		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	94
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	91
4			Triacontane	422	C30H62	000638-68-6	91
5			Octacosane	394	C28H58	000630-02-4	91

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	44.2	ng	2846720	1	6.75	1288570	20.0
3-Chloro-6-fluoro...	6.52	26.8	ng	1727210	1	6.75	1288570	20.0
1,2-Dichlorobenze...	6.90	57.4	ng	3699540	1	6.75	1288570	20.0
5,5,8a-Trimethyld...	11.16	4.1	ng	417535	4	11.29	2055340	20.0
5-Eicosene, (E)-	13.82	5.6	ng	657578	5	13.96	2362550	20.0
Heptacosane	15.10	2.2	ng	209077	6	15.44	1944450	20.0