LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000653.D
Acq On : 11 Oct 2019 23:58
Operator : JU
Sample : K5292-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId :

Integration Parameters: rteint.p
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 >
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	4.987	481	493	496	rBV	4484768	10912950	100.00%	22.790%
2	5.369	555	558	574	rVB	581374	608194	5.57%	1.270%
3	6.387	727	731	741	rBV	1949504	1782228	16.33%	3.722%
4	6.516	750	753	758	rBV	1079458	898483	8.23%	1.876%
5	6.746	789	792	796	rBV	1565628	1325242	12.14%	2.768%
6	6.905	815	819	822	rBV	4469597	3506964	32.14%	7.324%
7	7.310	882	888	891	rBV	2786903	2338395	21.43%	4.883%
8	7.416	903	906	910	rVB	260053	208011	1.91%	0.434%
9	7.457	910	913	916	rBV	241119	180496	1.65%	0.377%
10	8.034	1007	1011	1013	rBV	2121870	1710161	15.67%	3.571%
11	9.116	1191	1195	1198	rBV	6037465	4783328	43.83%	9.989%
12	9.510	1259	1262	1265	rBV	1201753	886868	8.13%	1.852%
13	9.799	1307	1311	1314	rBV	2630582	2147192	19.68%	4.484%
14	10.587	1442	1445	1452	rBV	463397	440910	4.04%	0.921%
15	11.157	1538	1542	1555	rVB	326256	350725	3.21%	0.732%
16	11.293	1561	1565	1568	rBV	2772775	2324867	21.30%	4.855%
17	11.363	1574	1577	1581	rVB2	138397	131131	1.20%	0.274%
18	12.522	1770	1774	1777	rVB	142891	130031	1.19%	0.272%
19	12.751	1809	1813	1816	rVB	158282	155662	1.43%	0.325%
20	12.898	1834	1838	1842	rBV	6009686	5509206	50.48%	11.505%
21	13.816	1991	1994	2009	rVB3	568360	796714	7.30%	1.664%
22	13.963	2015	2019	2023	rBV	2400020	2366011	21.68%	4.941%
23	14.145	2047	2050	2054	rBV	162934	148852	1.36%	0.311%
24	14.457	2100	2103	2106	rBV	241603	230593	2.11%	0.482%
25	14.763	2152	2155	2162	rVB	291434	307201	2.82%	0.642%
26	15.010	2194	2197	2200	rBV	79089	109351	1.00%	0.228%
27	15.104	2209	2213	2220	rVB2	323891	380696	3.49%	0.795%
28	15.375	2256	2259	2264	rVV	89276	119532	1.10%	0.250%
29	15.439	2265	2270	2274	rVV	1799852	2204113	20.20%	4.603%
30	15.486	2274	2278	2293	rVB2	287734	433252	3.97%	0.905%
31	15.928	2348	2353	2358	rBV	203164	314386	2.88%	0.657%
32	16.433	2435	2439	2444	rBV	89445	143376	1.31%	0.299%

LSC Area Percent Report

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Misc :
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Instrument :
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Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
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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_P\METHODS\8270-BP100119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

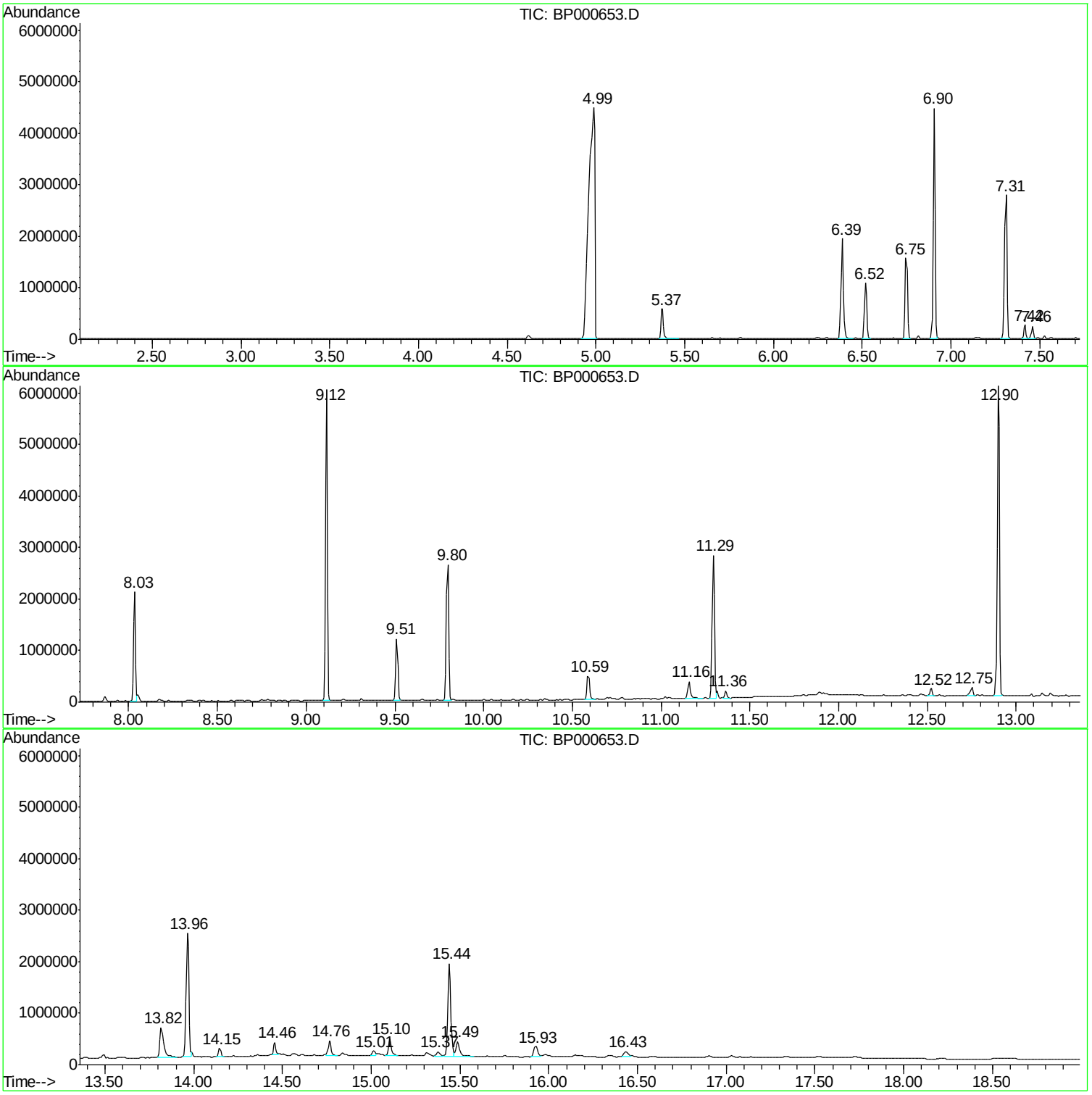
Sum of corrected areas: 47885121

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000653.D
Acq On : 11 Oct 2019 23:58
Operator : JU
Sample : K5292-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	164.69 ng	10913000	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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	13.56 ng	898483	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	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.90	52.93 ng	3506960	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	91
3	Benzenamine, N,N-dimethyl-4-nitr...	150	C8H10N2O	000138-89-6	32
4	2-Cyclohexene-1,4-dione, 5,6-dic...	370	C15H12Cl2N2O5	324051-56-1	12
5	2,5-Cyclohexadiene-1,4-dione, 5-...	334	C15H11ClN2O5	324051-61-8	12

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Peak Number 4 Benzene, 2-fluoro-1,3,5-tri... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.

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Operator : JU
Sample : K5292-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId :

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	2.43 ng	208011	Naphthalene-d8	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-fluoro-1,3,5-trimethyl-	138	C9H11F	000392-69-8	53
2	5-t-Butyl-4-methylimidazole	138	C8H14N2	146979-50-2	53
3	1-(2,4-Dimethyl-furan-3-yl)-etha...	138	C8H10O2	032933-07-6	52
4	Ethanone, 1-(3-fluorophenyl)-	138	C8H7FO	000455-36-7	52
5	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	50

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Peak Number 5 1,2-Benzenediol, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	2.11 ng	180496	Naphthalene-d8	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	50
2	Benzene	78	C6H6	000071-43-2	9
3	Fumaronitrile	78	C4H2N2	000764-42-1	9
4	2,4-Hexadiyne	78	C6H6	002809-69-0	7
5	Propanedinitrile, methylene-	78	C4H2N2	000922-64-5	7

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Peak Number 6 5-Caranol, trans,trans-(+)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	3.02 ng	350725	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Caranol, trans,trans-(+)-	154	C10H18O	006909-22-4	32
2	1-Methyl-3-n-propyl-2-pyrazolin-...	140	C7H12N2O	031272-04-5	27
3	5,5,8a-Trimethyldecalin-1-one	194	C13H22O	1000195-96-1	25
4	Acetamide, N-(2-fluorophenyl)-	153	C8H8FNO	000399-31-5	18
5	Cyclohexanone, 3-(4-hydroxybutyl...	184	C11H20O2	091212-98-5	16

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Peak Number 7 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	6.73 ng	796714	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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Acq On : 11 Oct 2019 23:58
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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId :

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Cyclopentadecane	210	C15H30	000295-48-7	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	1-Heptacosanol	396	C27H56O	002004-39-9	95
5	E-14-Hexadecenal	238	C16H30O	330207-53-9	94

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Peak Number 8 Hexatriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	2.79 ng	307201	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	93
2	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
5	Hexacosane	366	C26H54	000630-01-3	91

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Peak Number 9 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	3.45 ng	380696	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	95
2	Heneicosane	296	C21H44	000629-94-7	91
3	Docosane, 5-butyl-	366	C26H54	055282-16-1	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91

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Peak Number 10 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.85 ng	314386	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Docosane	310	C22H46	000629-97-0	87
3	Hexadecane	226	C16H34	000544-76-3	87

Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP101119\
Data File : BP000653.D
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Sample : K5292-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

4	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	87
5	Hexacosane	366 C26H54	000630-01-3	87

Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	164.7	ng	10913000	1	6.75	1325240	20.0
3-Chloro-6-fluoro...	6.52	13.6	ng	898483	1	6.75	1325240	20.0
1,2-Dichlorobenze...	6.90	52.9	ng	3506960	1	6.75	1325240	20.0
Benzene, 2-fluoro...	7.42	2.4	ng	208011	2	8.03	1710160	20.0
1,2-Benzenediol, ...	7.46	2.1	ng	180496	2	8.03	1710160	20.0
5-Caranol, trans,...	11.16	3.0	ng	350725	4	11.29	2324870	20.0
5-Eicosene, (E)-	13.82	6.7	ng	796714	5	13.96	2366010	20.0
Hexatriacontane	14.76	2.8	ng	307201	6	15.44	2204110	20.0
Tetracosane	15.10	3.5	ng	380696	6	15.44	2204110	20.0
Heneicosane	15.93	2.9	ng	314386	6	15.44	2204110	20.0