LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102220\
Data File : BF122088.D
Acq On : 22 Oct 2020 17:31
Operator : JU/CG
Sample : L4436-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 33B

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122088.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.945	482	486	496	rBV	25251	42415	1.69%	0.203%
2	5.351	552	555	583	rBV	2068883	2252097	89.67%	10.803%
3	6.381	726	730	752	rBV	2202890	2310718	92.00%	11.084%
4	6.587	763	765	777	rBV	20981	46914	1.87%	0.225%
5	6.728	786	789	797	rVB	781559	641771	25.55%	3.078%
6	7.298	882	886	905	rBV	1714663	1596319	63.56%	7.657%
7	8.010	1004	1007	1027	rVB	903439	881787	35.11%	4.230%
8	9.086	1185	1190	1200	rBV	2555018	2511582	100.00%	12.047%
9	9.204	1205	1210	1217	rVB2	17954	28882	1.15%	0.139%
10	9.480	1254	1257	1265	rVB	314864	292198	11.63%	1.402%
11	9.757	1301	1304	1308	rBV	967459	903824	35.99%	4.335%
12	9.792	1308	1310	1318	rVB	44037	41989	1.67%	0.201%
13	10.310	1395	1398	1403	rVB	32755	29961	1.19%	0.144%
14	10.551	1435	1439	1455	rBV	1523574	1526879	60.79%	7.324%
15	10.669	1455	1459	1464	rVB4	16693	29037	1.16%	0.139%
16	10.845	1485	1489	1494	rBV	98142	94793	3.77%	0.455%
17	11.245	1553	1557	1559	rBV	955482	823891	32.80%	3.952%
18	11.269	1559	1561	1567	rVV	350058	322363	12.84%	1.546%
19	11.322	1567	1570	1577	rVB	62484	80296	3.20%	0.385%
20	11.492	1594	1599	1603	rBV	37670	43635	1.74%	0.209%
21	11.751	1639	1643	1645	rBV	32343	31961	1.27%	0.153%
22	11.774	1645	1647	1654	rVB3	68790	72726	2.90%	0.349%
23	11.857	1658	1661	1664	rBV	40543	45951	1.83%	0.220%
24	12.457	1760	1763	1769	rBV	381253	356137	14.18%	1.708%
25	12.686	1797	1802	1807	rBV	313598	347722	13.84%	1.668%
26	12.827	1822	1826	1829	rBV	2318531	1963259	78.17%	9.417%
27	12.868	1829	1833	1836	rVB2	25356	32623	1.30%	0.156%
28	12.904	1836	1839	1845	rVB2	21303	33578	1.34%	0.161%
29	12.957	1845	1848	1851	rBV2	43381	38462	1.53%	0.184%
30	12.998	1851	1855	1856	rBV2	26546	33407	1.33%	0.160%
31	13.016	1856	1858	1861	rVB	31635	30883	1.23%	0.148%
32	13.051	1861	1864	1867	rBV2	38080	38782	1.54%	0.186%
33	13.121	1872	1876	1881	rVB3	33842	44049	1.75%	0.211%
34	13.251	1894	1898	1900	rBV2	18129	28317	1.13%	0.136%
35	13.392	1919	1922	1925	rBV3	34542	39170	1.56%	0.188%
36	13.539	1944	1947	1953	rVB	31058	36472	1.45%	0.175%

LSC Area Percent Report

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Operator : JU/CG
Sample : L4436-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 33B

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.639	1962	1964	1966	rBV2	31330	26196	1.04%	0.126%
38	13.733	1976	1980	1988	rBV4	137709	299269	11.92%	1.435%
39	13.792	1988	1990	1997	rVB2	46279	52282	2.08%	0.251%
40	13.857	1997	2001	2002	rBV	130052	121003	4.82%	0.580%
41	13.886	2002	2006	2009	rVV2	824684	876526	34.90%	4.204%
42	13.915	2009	2011	2018	rVB	186188	174471	6.95%	0.837%
43	14.339	2081	2083	2087	rBV3	52943	61198	2.44%	0.294%
44	14.498	2108	2110	2113	rBV	41672	36672	1.46%	0.176%
45	14.915	2177	2181	2183	rBV	137211	180518	7.19%	0.866%
46	15.204	2227	2230	2233	rBV	78080	81869	3.26%	0.393%
47	15.262	2237	2240	2244	rVB	121548	135232	5.38%	0.649%
48	15.321	2245	2250	2254	rBV	566413	688039	27.39%	3.300%
49	15.504	2278	2281	2284	rBV3	38623	49911	1.99%	0.239%
50	15.945	2353	2356	2364	rVB3	75637	123023	4.90%	0.590%
51	16.739	2487	2491	2499	rVB2	89808	171573	6.83%	0.823%
52	16.892	2513	2517	2523	rVB6	47604	95243	3.79%	0.457%

Sum of corrected areas: 20847875

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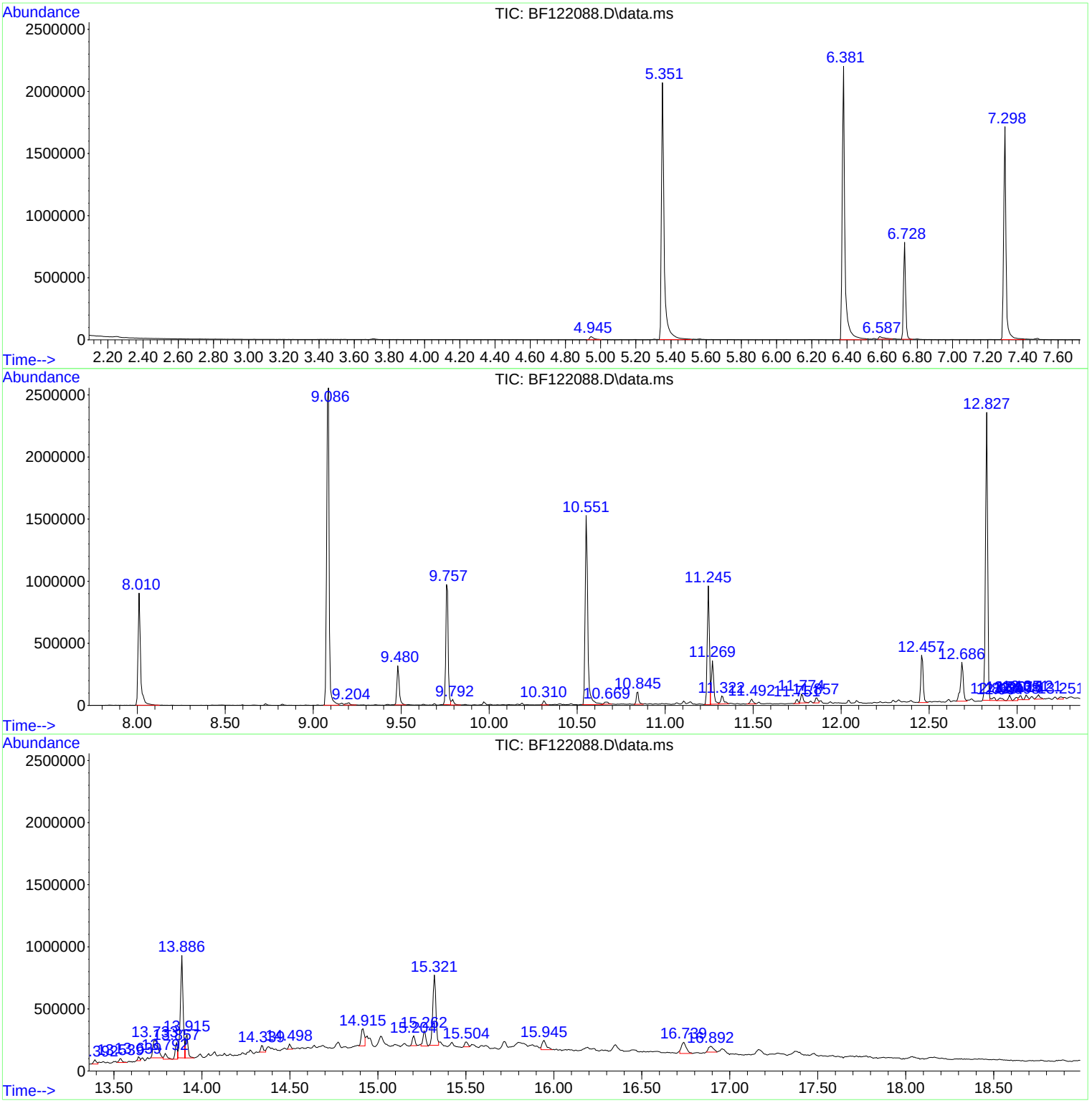
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
33B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102220\
Data File : BF122088.D
Acq On : 22 Oct 2020 17:31
Operator : JU/CG
Sample : L4436-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 33B

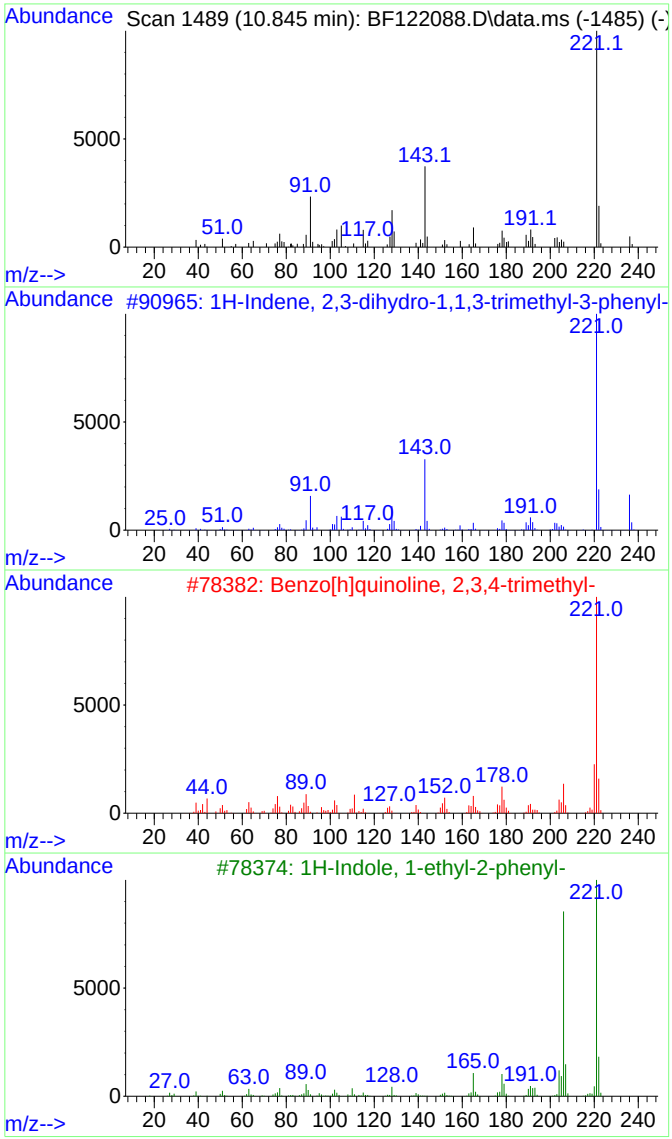
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

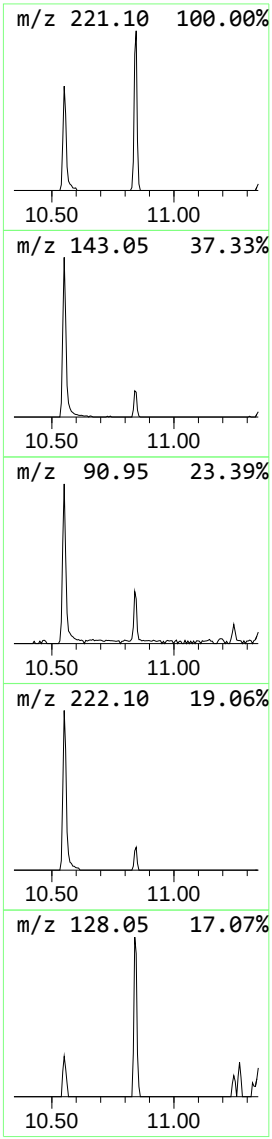
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.845	2.30 ng	94793	Phenanthrene-d10	11.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	86
2	Benzo[h]quinoline, 2,3,4-trimethyl-	221	C16H15N	063042-66-0	58
3	1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	53
4	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	50
5	4,6-Dimethyl-2-thioxo-1,2-dihydr...	236	C11H16N2SSi	1000332-43-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102220\
Data File : BF122088.D
Acq On : 22 Oct 2020 17:31
Operator : JU/CG
Sample : L4436-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 33B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

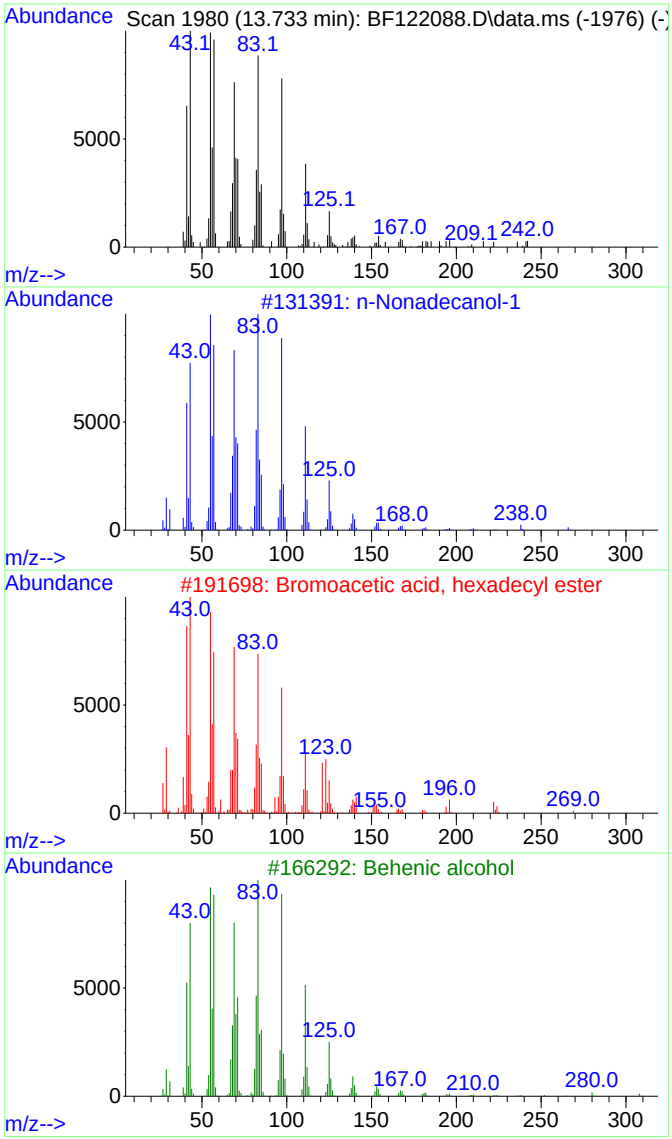
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

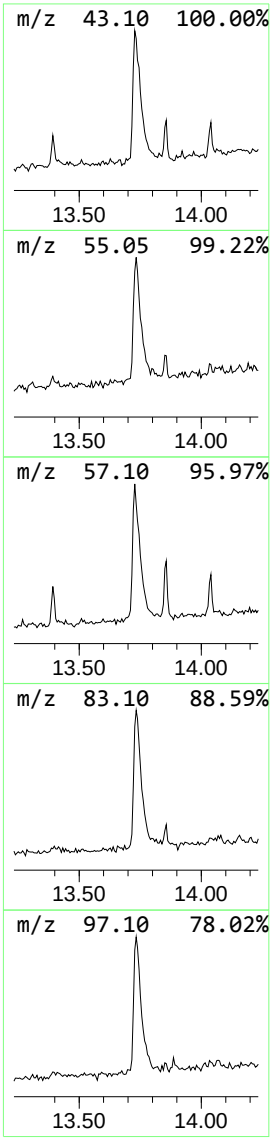
****

Peak Number 2 n-Nonadecanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	6.83 ng	299269	Chrysene-d12	13.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Cyclotridecane	182	C13H26	000295-02-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102220\
Data File : BF122088.D
Acq On : 22 Oct 2020 17:31
Operator : JU/CG
Sample : L4436-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 33B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

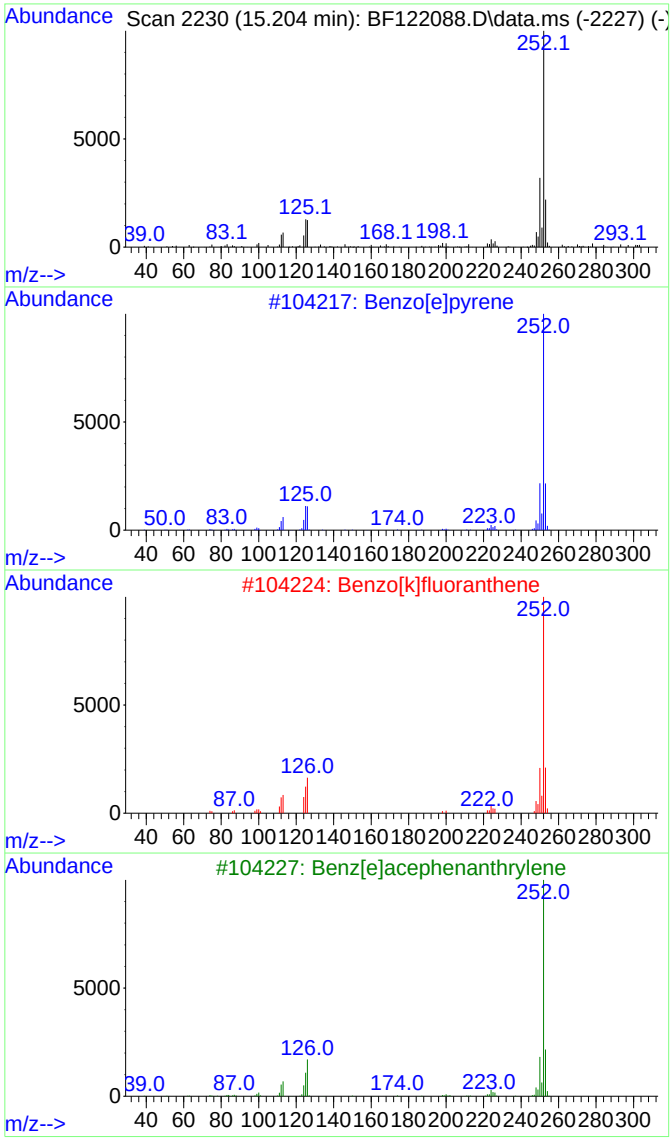
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

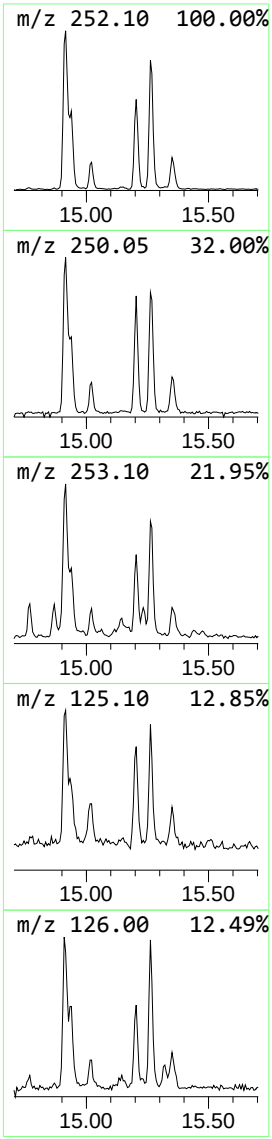
****

Peak Number 3 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	2.38 ng	81869	Perylene-d12	15.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	96
5	Perylene	252	C20H12	000198-55-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102220\
Data File : BF122088.D
Acq On : 22 Oct 2020 17:31
Operator : JU/CG
Sample : L4436-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 33B

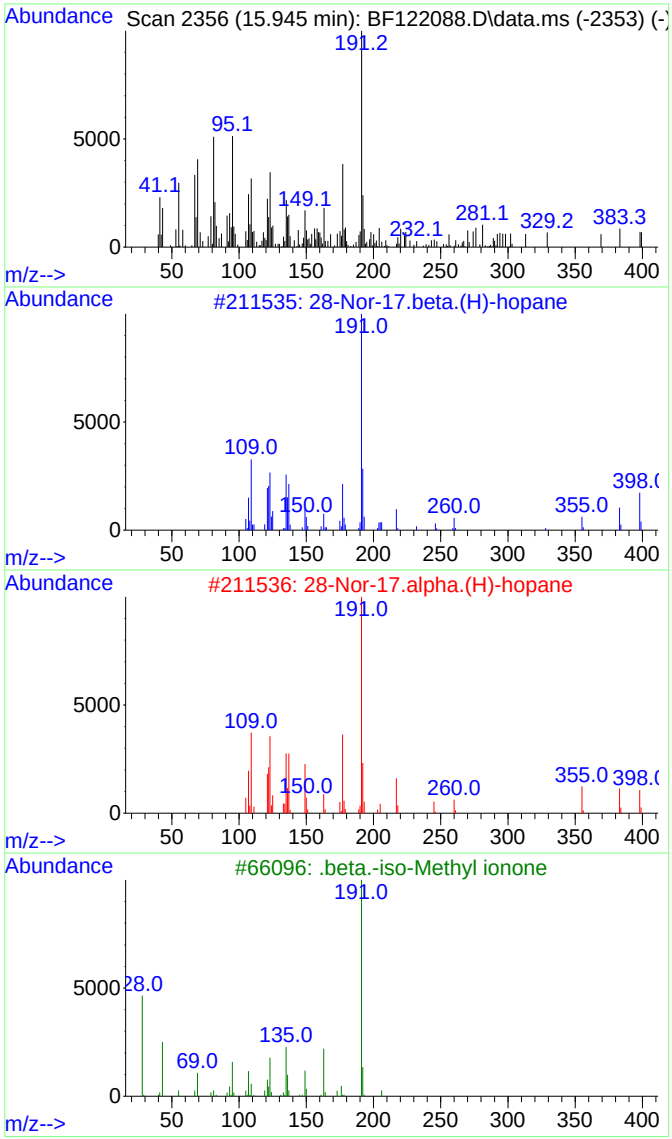
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

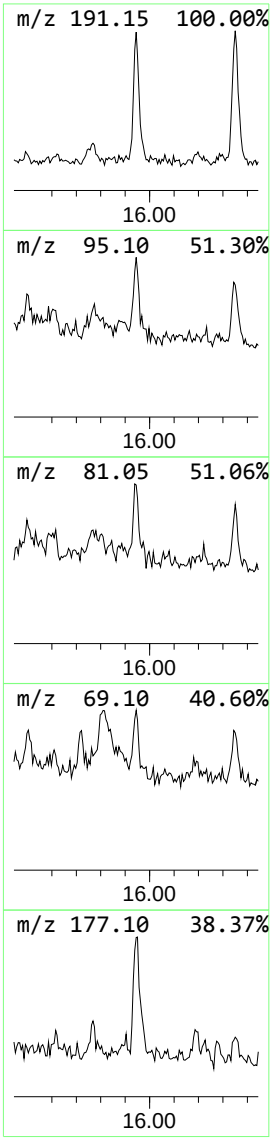
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 28-Nor-17.beta.(H)-hopane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	3.58 ng	123023	Perylene-d12	15.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	53
2	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	49
3	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43
4	5-(7a-Isopropenyl-4,5-dimethyl-o...	290	C20H34O	1000193-54-0	42
5	5-(1-Isopropenyl-4,5-dimethylbic...	332	C22H36O2	1000195-69-8	38





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Acq On : 22 Oct 2020 17:31
Operator : JU/CG
Sample : L4436-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 33B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

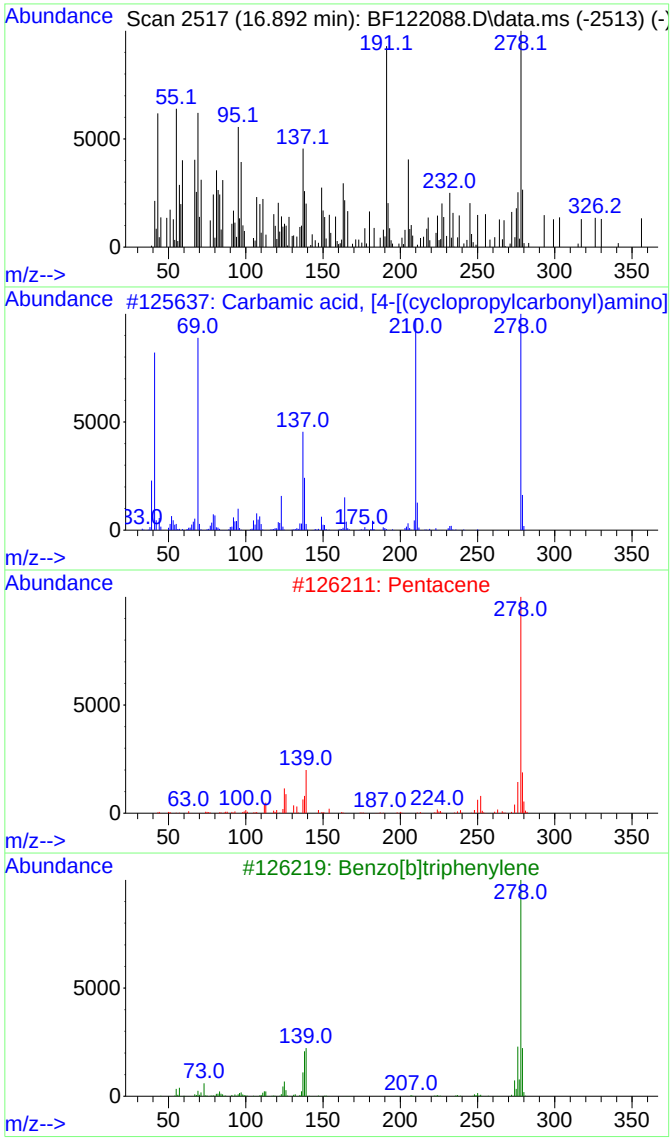
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

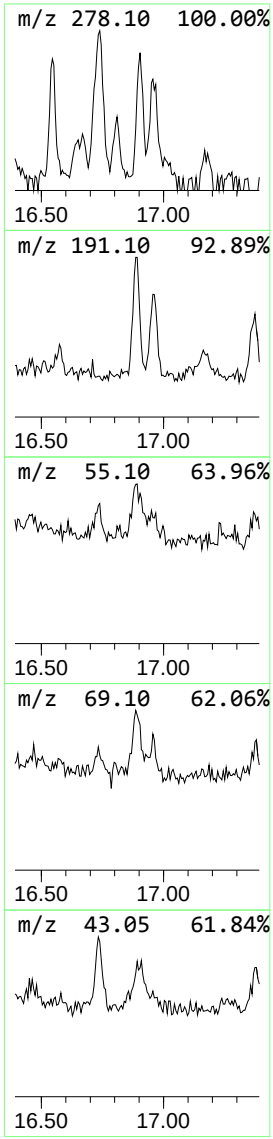
****

Peak Number 5 unknown16.89 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.892	2.77 ng	95243	Perylene-d12	15.321

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbamic acid, [4-[(cyclopropylc...	278	C14H18N2O4	1000337-41-0	25
2	Pentacene	278	C22H14	000135-48-8	25
3	Benzo[b]triphenylene	278	C22H14	000215-58-7	18
4	Anthracene, 1-(3-butenyl)-	232	C18H16	1000156-51-8	14
5	2-Fluoro-4-(trifluoromethyl)acet...	206	C9H6F4O	122023-29-4	11





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1H-Indene, 2,3-...	10.845	2.3	ng	94793	4	11.245	823891	20.0
n-Nonadecanol-1	13.733	6.8	ng	299269	5	13.886	876526	20.0
Benzo[e]pyrene	15.204	2.4	ng	81869	6	15.321	688039	20.0
28-Nor-17.beta....	15.945	3.6	ng	123023	6	15.321	688039	20.0
unknown16.89	16.892	2.8	ng	95243	6	15.321	688039	20.0