LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125879.D
Acq On : 18 Oct 2021 16:12
Operator : JU/CG
Sample : M4249-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-(D)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125879.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.439	565	570	573	rBV	3193931	2968670	81.51%	9.871%
2	6.451	737	742	745	rBV	2960302	2918506	80.13%	9.704%
3	6.822	802	805	808	rBV	1227553	936304	25.71%	3.113%
4	7.381	895	900	903	rBV	2121564	1884578	51.75%	6.266%
5	8.004	1003	1006	1014	rBV	271834	209951	5.76%	0.698%
6	8.104	1017	1023	1025	rBV	1638471	1330135	36.52%	4.423%
7	8.122	1025	1026	1032	rVB	130801	95031	2.61%	0.316%
8	8.816	1140	1144	1148	rVB	144963	123151	3.38%	0.409%
9	8.910	1157	1160	1164	rVB	151280	135541	3.72%	0.451%
10	9.180	1201	1206	1209	rBV	3812646	3642011	100.00%	12.110%
11	9.274	1221	1222	1229	rVB2	46091	36773	1.01%	0.122%
12	9.439	1246	1250	1254	rBV	85771	109206	3.00%	0.363%
13	9.516	1259	1263	1265	rVV	141039	137849	3.78%	0.458%
14	9.539	1265	1267	1270	rVV	104661	76627	2.10%	0.255%
15	9.580	1270	1274	1280	rVB5	37968	46305	1.27%	0.154%
16	9.627	1280	1282	1288	rBV	59496	67096	1.84%	0.223%
17	9.716	1293	1297	1302	rBV	88885	79694	2.19%	0.265%
18	9.857	1314	1321	1324	rBV	1684345	1503729	41.29%	5.000%
19	9.886	1324	1326	1330	rVB2	119205	92887	2.55%	0.309%
20	10.057	1351	1355	1359	rVB	160248	131339	3.61%	0.437%
21	10.098	1359	1362	1368	rVB	47092	46995	1.29%	0.156%
22	10.169	1368	1374	1377	rBV2	37008	40210	1.10%	0.134%
23	10.263	1385	1390	1391	rBV2	32027	38318	1.05%	0.127%
24	10.398	1410	1413	1419	rVB	277834	245510	6.74%	0.816%
25	10.557	1437	1440	1444	rVB	49712	43759	1.20%	0.145%
26	10.639	1450	1454	1458	rBV	2258053	1959403	53.80%	6.515%
27	10.763	1471	1475	1479	rBV4	33008	44772	1.23%	0.149%
28	10.945	1499	1506	1509	rBV2	63041	74883	2.06%	0.249%
29	11.233	1553	1555	1560	rVB	83733	64288	1.77%	0.214%
30	11.339	1569	1573	1575	rBV	1367050	1278990	35.12%	4.253%
31	11.363	1575	1577	1580	rVV	1055835	775358	21.29%	2.578%
32	11.410	1580	1585	1588	rVB	214213	191363	5.25%	0.636%
33	11.563	1605	1611	1614	rBV2	71860	64406	1.77%	0.214%
34	11.839	1652	1658	1660	rBV	153145	137357	3.77%	0.457%
35	11.863	1660	1662	1666	rVV	254441	223048	6.12%	0.742%
36	11.910	1666	1670	1673	rVV2	52132	56236	1.54%	0.187%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125879.D
Acq On : 18 Oct 2021 16:12
Operator : JU/CG
Sample : M4249-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-(D)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.951	1673	1677	1679	rVV2	189342	207715	5.70%	0.691%
38	11.968	1679	1680	1685	rVB	90753	72087	1.98%	0.240%
39	12.133	1705	1708	1710	rBV	67431	53008	1.46%	0.176%
40	12.386	1747	1751	1754	rBV	75622	72465	1.99%	0.241%
41	12.421	1754	1757	1759	rVV3	44711	53714	1.47%	0.179%
42	12.468	1763	1765	1770	rBV3	31999	42114	1.16%	0.140%
43	12.545	1775	1778	1782	rVB	611918	491298	13.49%	1.634%
44	12.645	1792	1795	1798	rBV2	42077	41100	1.13%	0.137%
45	12.774	1811	1817	1820	rBV	554182	512638	14.08%	1.705%
46	12.827	1823	1826	1830	rVB3	27825	38009	1.04%	0.126%
47	12.921	1838	1842	1845	rVB	2813722	2477703	68.03%	8.238%
48	12.992	1850	1854	1857	rBV3	41754	64188	1.76%	0.213%
49	13.104	1870	1873	1876	rVB	103598	93321	2.56%	0.310%
50	13.168	1876	1884	1887	rBV	91056	97040	2.66%	0.323%
51	13.210	1887	1891	1894	rVV2	64785	64602	1.77%	0.215%
52	13.298	1903	1906	1909	rVB	45084	37154	1.02%	0.124%
53	13.327	1909	1911	1915	rBV	43749	42222	1.16%	0.140%
54	13.604	1956	1958	1963	rVB	29609	38737	1.06%	0.129%
55	13.721	1973	1978	1980	rBV2	42442	57655	1.58%	0.192%
56	13.815	1991	1994	2004	rVB5	73307	106981	2.94%	0.356%
57	13.968	2015	2020	2023	rBV2	1211816	1270120	34.87%	4.223%
58	13.998	2023	2025	2030	rVB	202680	184049	5.05%	0.612%
59	14.357	2083	2086	2089	rVB	61881	56280	1.55%	0.187%
60	14.727	2145	2149	2156	rBV	325231	374686	10.29%	1.246%
61	14.821	2162	2165	2168	rBV2	39332	46923	1.29%	0.156%
62	14.998	2191	2195	2198	rBV	160571	234892	6.45%	0.781%
63	15.104	2211	2213	2219	rVB	44904	49149	1.35%	0.163%
64	15.298	2242	2246	2251	rVB	96617	124767	3.43%	0.415%
65	15.356	2252	2256	2261	rBV	139975	171582	4.71%	0.571%
66	15.421	2262	2267	2270	rBV	792498	933893	25.64%	3.105%
67	16.845	2505	2509	2516	rVB2	44436	83938	2.30%	0.279%
68	17.286	2577	2584	2588	rBV3	30974	70966	1.95%	0.236%

Sum of corrected areas: 30075275

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
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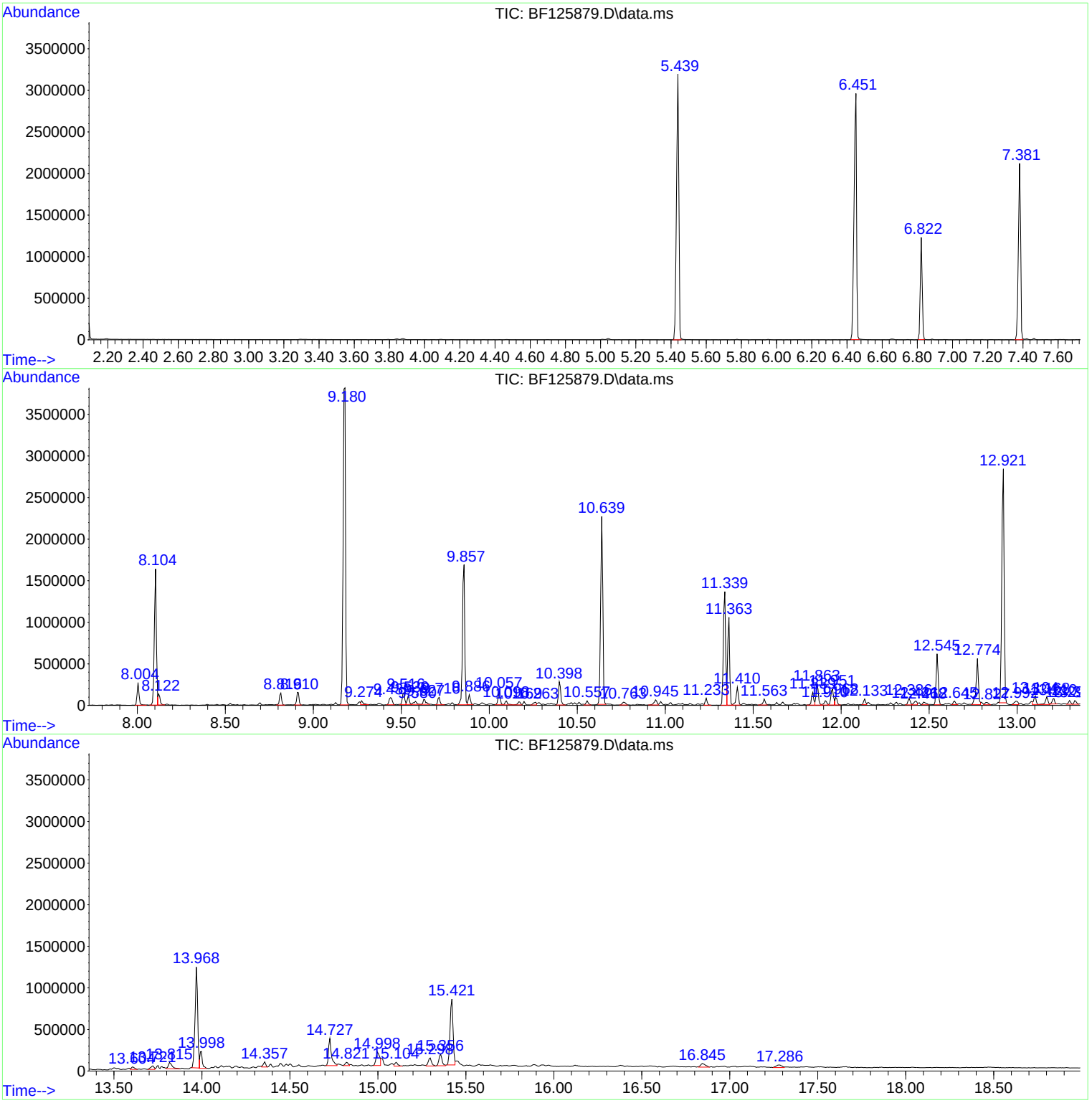
Acq On : 18 Oct 2021 16:12
Operator : JU/CG
Sample : M4249-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2-(D)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125879.D
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Operator : JU/CG
Sample : M4249-10
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BNA_F
ClientSampleId :
TP2-(D)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

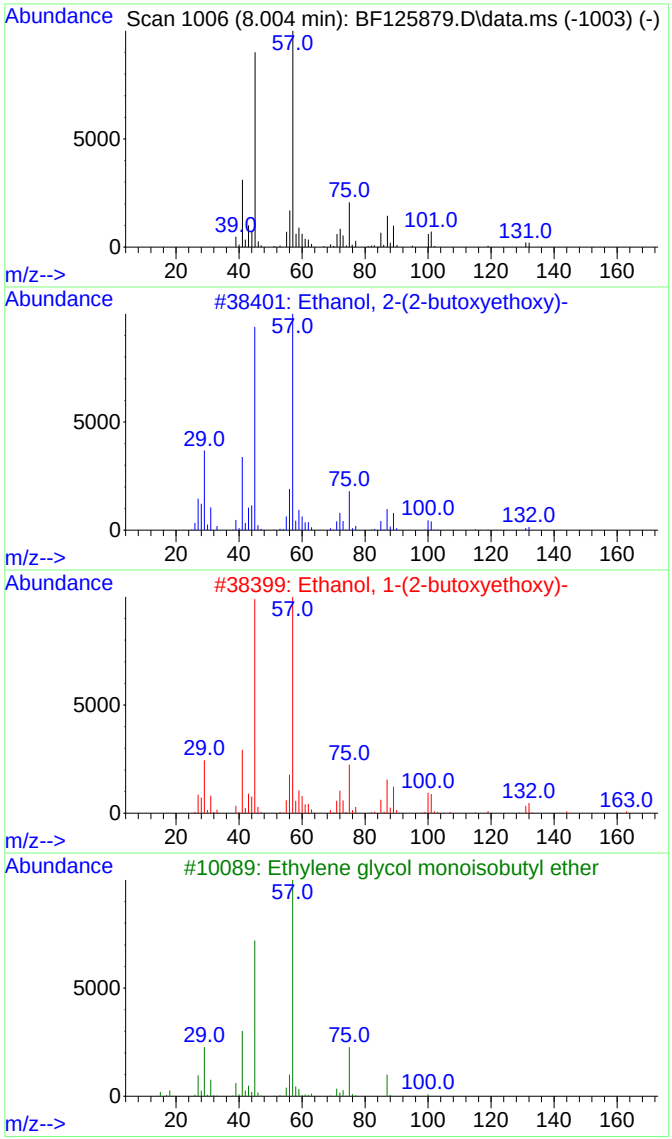
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

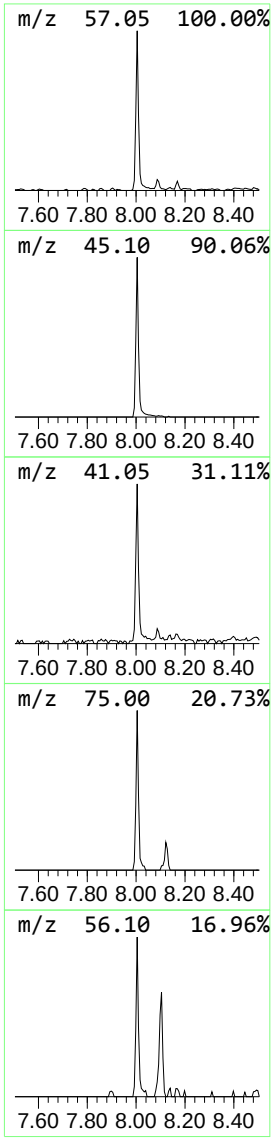
****

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	3.16 ng	209951	Naphthalene-d8	8.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125879.D
Acq On : 18 Oct 2021 16:12
Operator : JU/CG
Sample : M4249-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2-(D)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

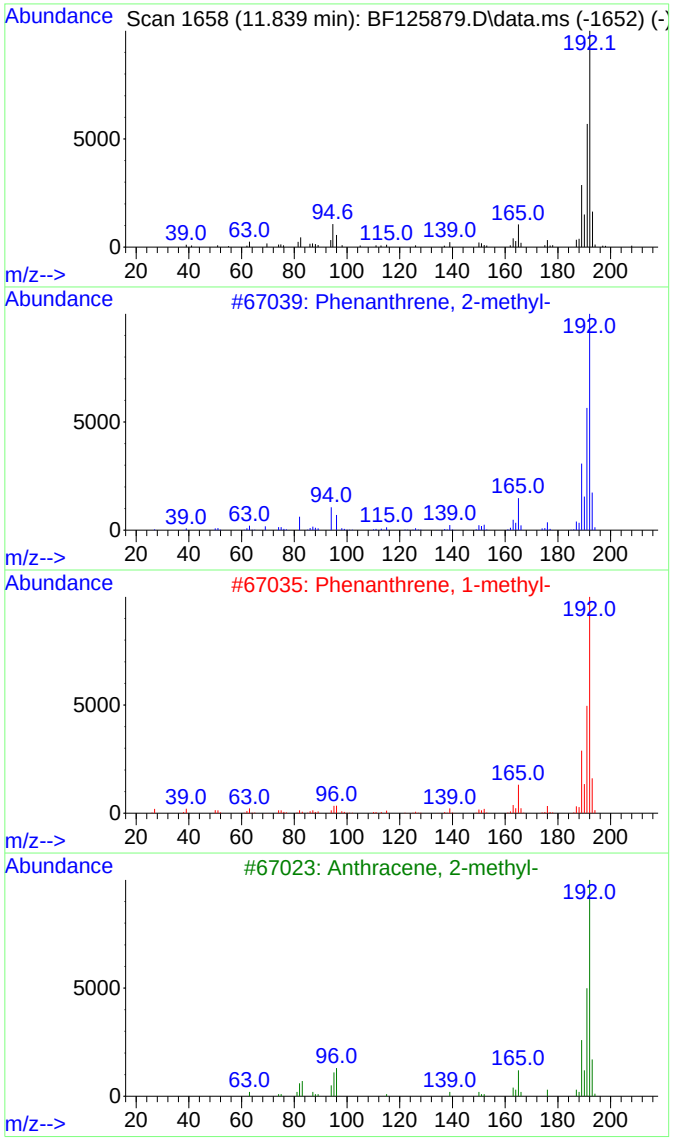
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

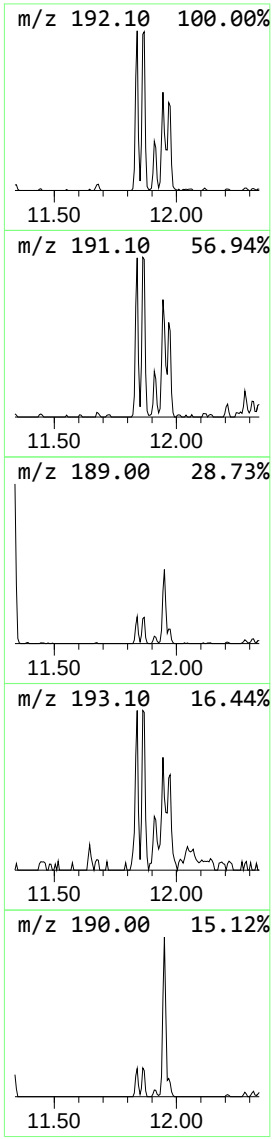
****

Peak Number 2 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	2.15 ng	137357	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
5	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125879.D
Acq On : 18 Oct 2021 16:12
Operator : JU/CG
Sample : M4249-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2-(D)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

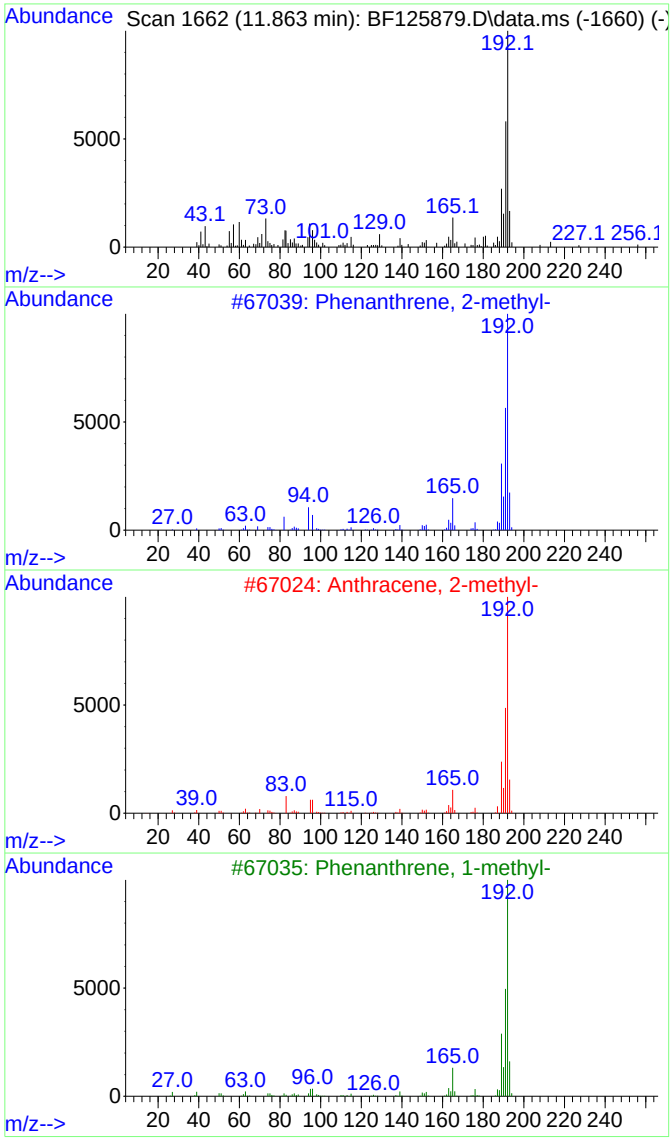
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

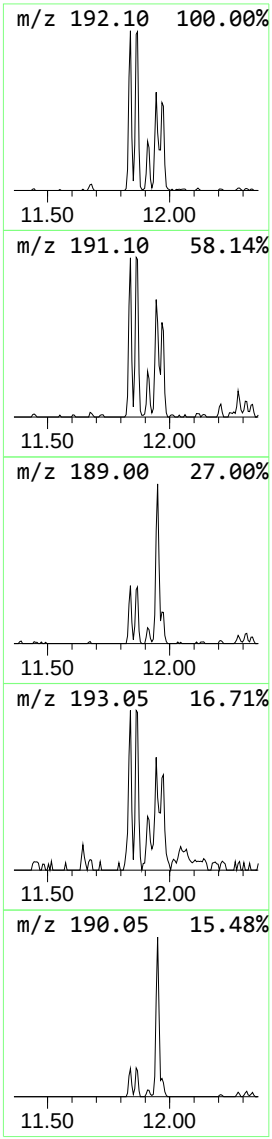
****

Peak Number 3 Anthracene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	3.49 ng	223048	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125879.D
Acq On : 18 Oct 2021 16:12
Operator : JU/CG
Sample : M4249-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2-(D)

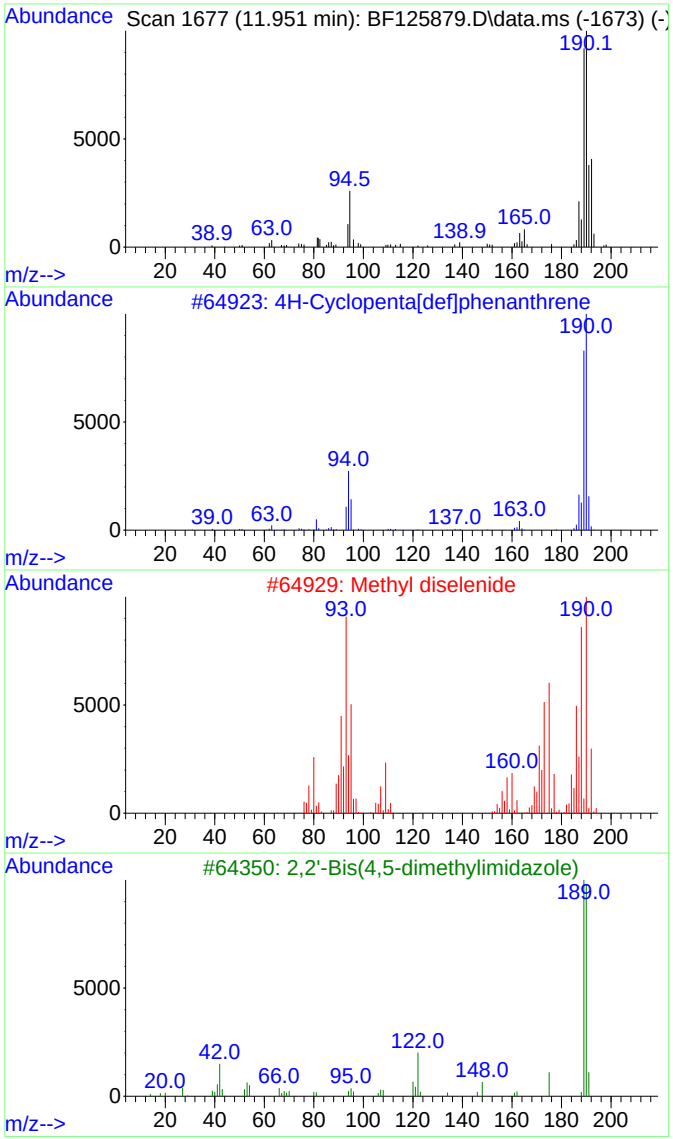
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

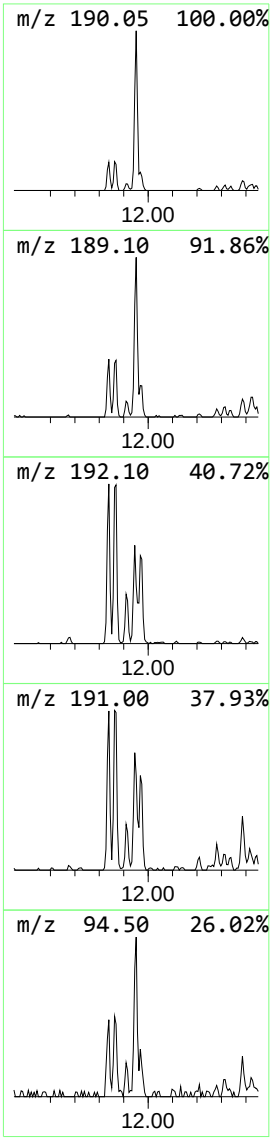
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	3.25 ng	207715	Phenanthrene-d10	11.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Methyl diselenide	190	C2H6Se2	007101-31-7	43
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
4	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	32
5	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125879.D
Acq On : 18 Oct 2021 16:12
Operator : JU/CG
Sample : M4249-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2-(D)

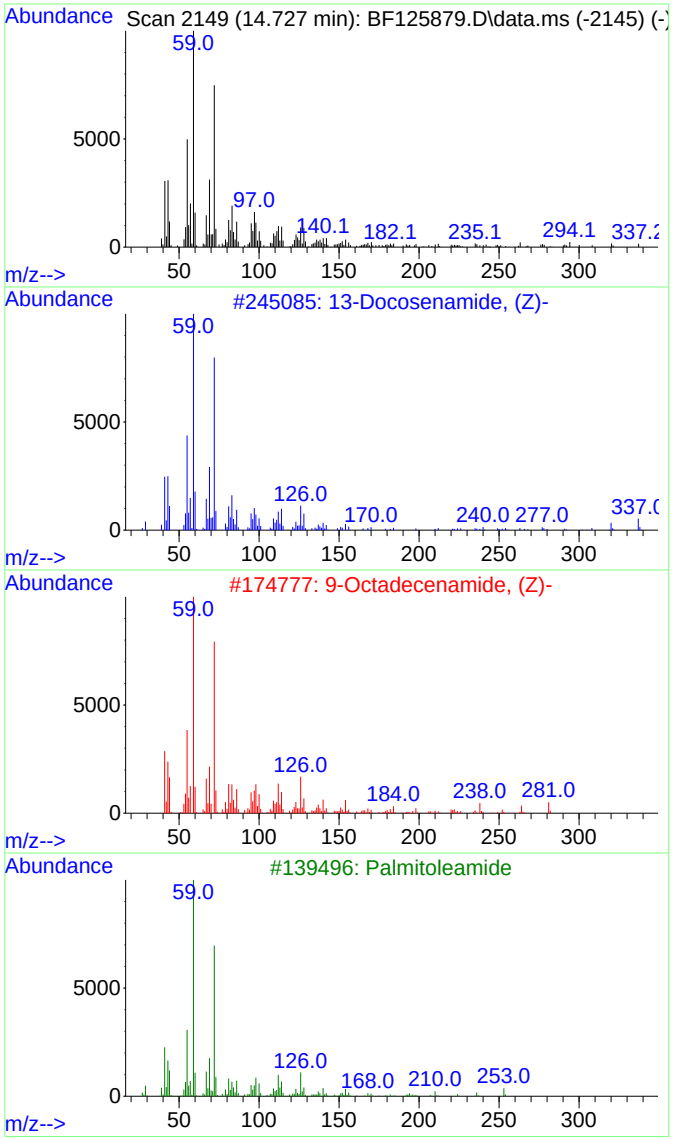
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

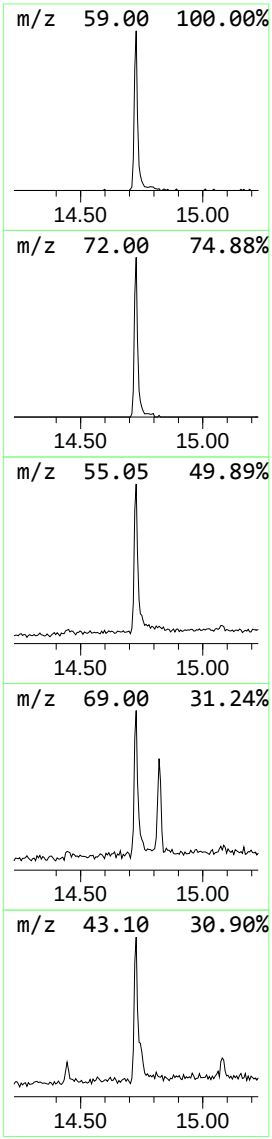
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	8.02 ng	374686	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	97
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	Palmitoleamide	253	C16H31NO	106010-22-4	59
4	Octadecanamide	283	C18H37NO	000124-26-5	43
5	Methyl 15-methoxyhexadecanoate	300	C18H36O3	1000110-17-9	35





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Data File : BF125879.D
Acq On : 18 Oct 2021 16:12
Operator : JU/CG
Sample : M4249-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP2-(D)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

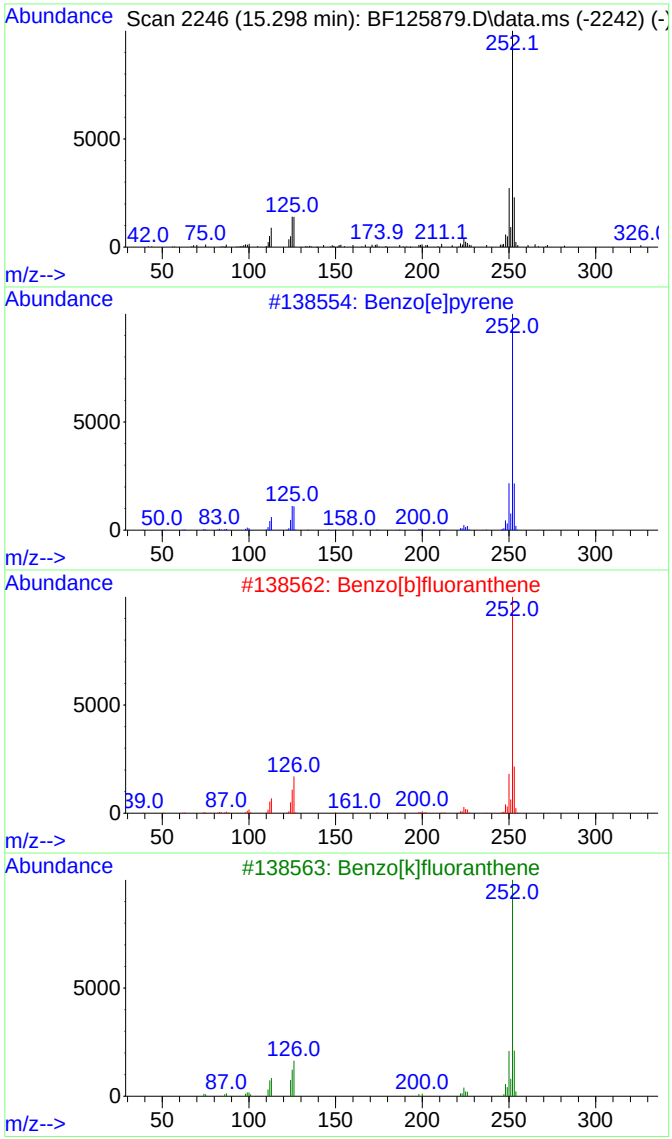
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

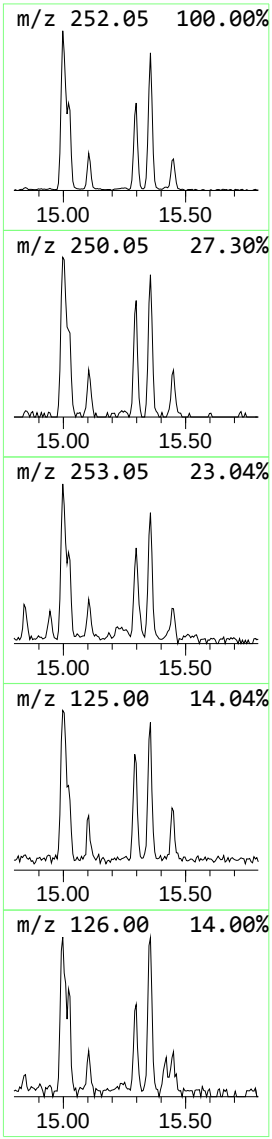
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	2.67 ng	124767	Perylene-d12	15.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
5	Benzo[a]pyrene	252	C20H12	000050-32-8	96





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101821\
Data File : BF125879.D
Acq On : 18 Oct 2021 16:12
Operator : JU/CG
Sample : M4249-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-(D)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.004	3.2	ng	209951	2	8.104	1330140	20.0
Phenanthrene, 2...	11.839	2.1	ng	137357	4	11.339	1278990	20.0
Anthracene, 2-m...	11.863	3.5	ng	223048	4	11.339	1278990	20.0
4H-Cyclopenta[d...	11.951	3.3	ng	207715	4	11.339	1278990	20.0
13-Docosenamide...	14.727	8.0	ng	374686	6	15.421	933893	20.0
Benzo[e]pyrene	15.298	2.7	ng	124767	6	15.421	933893	20.0