LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126065.D
Acq On : 8 Nov 2021 15:04
Operator : JU/CG
Sample : M4472-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-2-KS

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126065.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	5	13	23	rVB	1501929	1891988	42.45%	4.819%
2	5.081	505	509	515	rVB	45064	53603	1.20%	0.137%
3	5.475	571	576	579	rBV	4574112	4035546	90.54%	10.278%
4	6.481	741	747	750	rBV	4260453	4119520	92.42%	10.492%
5	6.851	807	810	814	rBV	1437657	1156707	25.95%	2.946%
6	7.416	900	906	909	rBV	2844267	2636991	59.16%	6.716%
7	8.034	1008	1011	1022	rBV	170859	193130	4.33%	0.492%
8	8.134	1024	1028	1032	rBV	1662867	1393539	31.26%	3.549%
9	9.210	1206	1211	1214	rBV	5629810	4457221	100.00%	11.352%
10	9.886	1322	1326	1330	rBV	1738981	1392693	31.25%	3.547%
11	10.433	1415	1419	1425	rVB	95832	91707	2.06%	0.234%
12	10.675	1456	1460	1463	rBV	2651980	2329038	52.25%	5.932%
13	10.804	1478	1482	1488	rVB5	40639	67879	1.52%	0.173%
14	11.269	1558	1561	1566	rVB2	66418	68924	1.55%	0.176%
15	11.369	1575	1578	1581	rBV	1299911	1278176	28.68%	3.255%
16	11.392	1581	1582	1586	rVV	750908	552404	12.39%	1.407%
17	11.445	1587	1591	1594	rVB	219461	199745	4.48%	0.509%
18	11.875	1661	1664	1666	rBV	84436	74153	1.66%	0.189%
19	11.898	1666	1668	1672	rVB	140347	117290	2.63%	0.299%
20	11.986	1679	1683	1685	rBV	247486	234440	5.26%	0.597%
21	12.169	1711	1714	1716	rBV	81861	68362	1.53%	0.174%
22	12.192	1716	1718	1724	rVB3	70441	72022	1.62%	0.183%
23	12.422	1755	1757	1761	rBV3	63914	82698	1.86%	0.211%
24	12.475	1761	1766	1769	rVB4	46471	83838	1.88%	0.214%
25	12.504	1769	1771	1778	rBV2	76174	112937	2.53%	0.288%
26	12.586	1781	1785	1788	rVB	1567494	1276679	28.64%	3.252%
27	12.816	1818	1824	1827	rBV	1319515	1318438	29.58%	3.358%
28	12.957	1844	1848	1852	rVB	4017581	3545117	79.54%	9.029%
29	13.033	1856	1861	1864	rBV2	82646	128015	2.87%	0.326%
30	13.116	1873	1875	1877	rBV2	46825	56301	1.26%	0.143%
31	13.139	1877	1879	1882	rVB	185295	152318	3.42%	0.388%
32	13.204	1888	1890	1893	rBV	93260	84944	1.91%	0.216%
33	13.245	1894	1897	1900	rVB2	115058	98625	2.21%	0.251%
34	13.333	1910	1912	1915	rBV	68481	59248	1.33%	0.151%
35	13.369	1915	1918	1921	rBV	71907	78788	1.77%	0.201%
36	13.498	1937	1940	1944	rBV	112830	116289	2.61%	0.296%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126065.D
Acq On : 8 Nov 2021 15:04
Operator : JU/CG
Sample : M4472-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-KS

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.645	1963	1965	1970	rVB	66346	67125	1.51%	0.171%
38	13.810	1991	1993	1997	rBV2	104970	107505	2.41%	0.274%
39	13.863	1998	2002	2008	rVB2	145771	230394	5.17%	0.587%
40	14.010	2022	2027	2030	rBV2	1462092	1852239	41.56%	4.718%
41	14.033	2030	2031	2037	rVB	575068	426482	9.57%	1.086%
42	14.116	2042	2045	2047	rBV	91077	67622	1.52%	0.172%
43	14.151	2049	2051	2055	rBV2	59369	63452	1.42%	0.162%
44	14.868	2170	2173	2181	rVB	293060	311294	6.98%	0.793%
45	15.051	2200	2204	2207	rBV	386560	601217	13.49%	1.531%
46	15.351	2252	2255	2260	rVB	241225	284182	6.38%	0.724%
47	15.410	2262	2265	2270	rBV	306762	346806	7.78%	0.883%
48	15.474	2272	2276	2279	rBV	685724	781419	17.53%	1.990%
49	16.927	2519	2523	2531	rVB2	129081	247424	5.55%	0.630%
50	17.368	2594	2598	2606	rVB	103246	196635	4.41%	0.501%

Sum of corrected areas: 39263109

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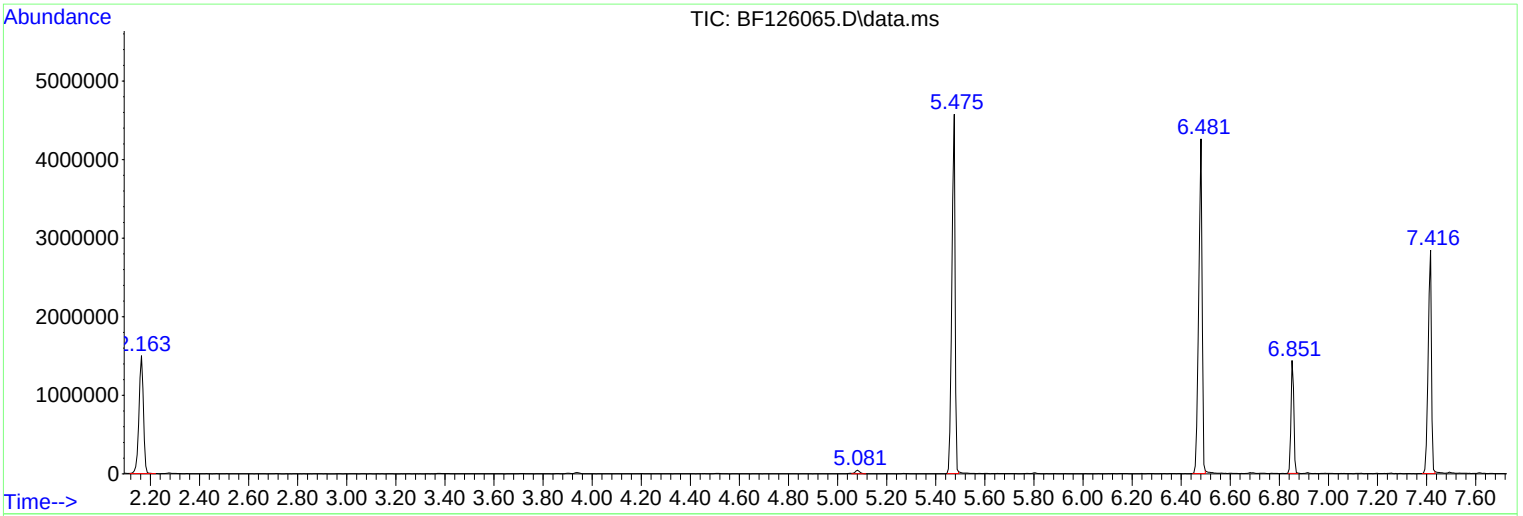
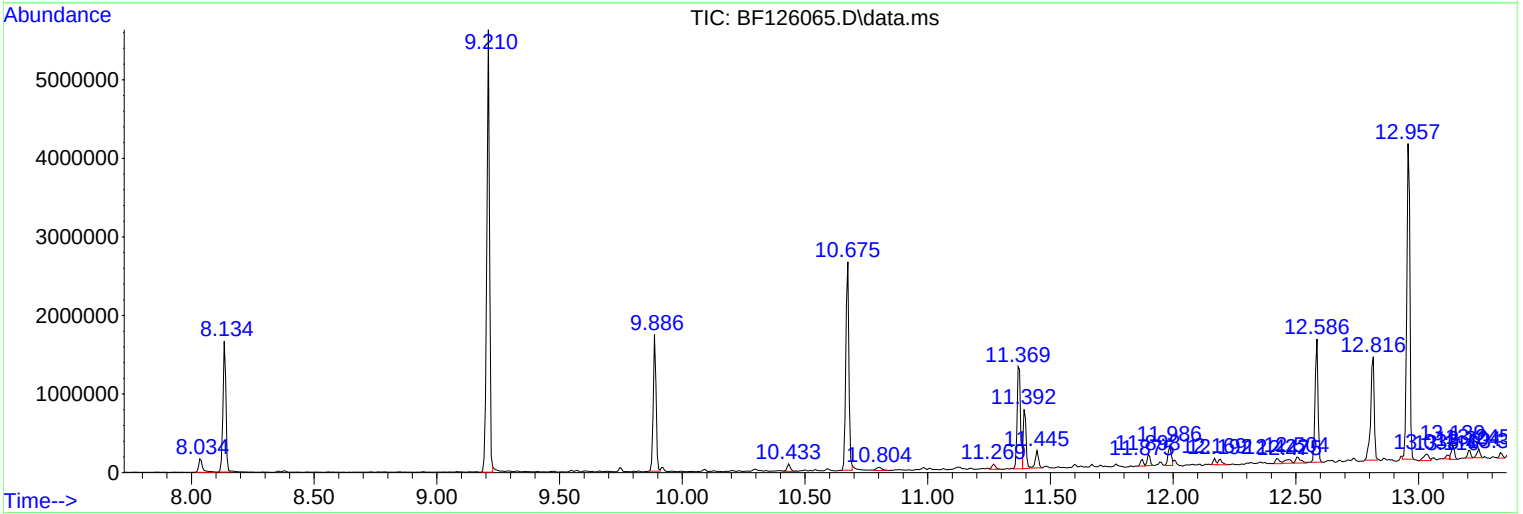
Misc :
ALS Vial : 10 Sample Multiplier: 1

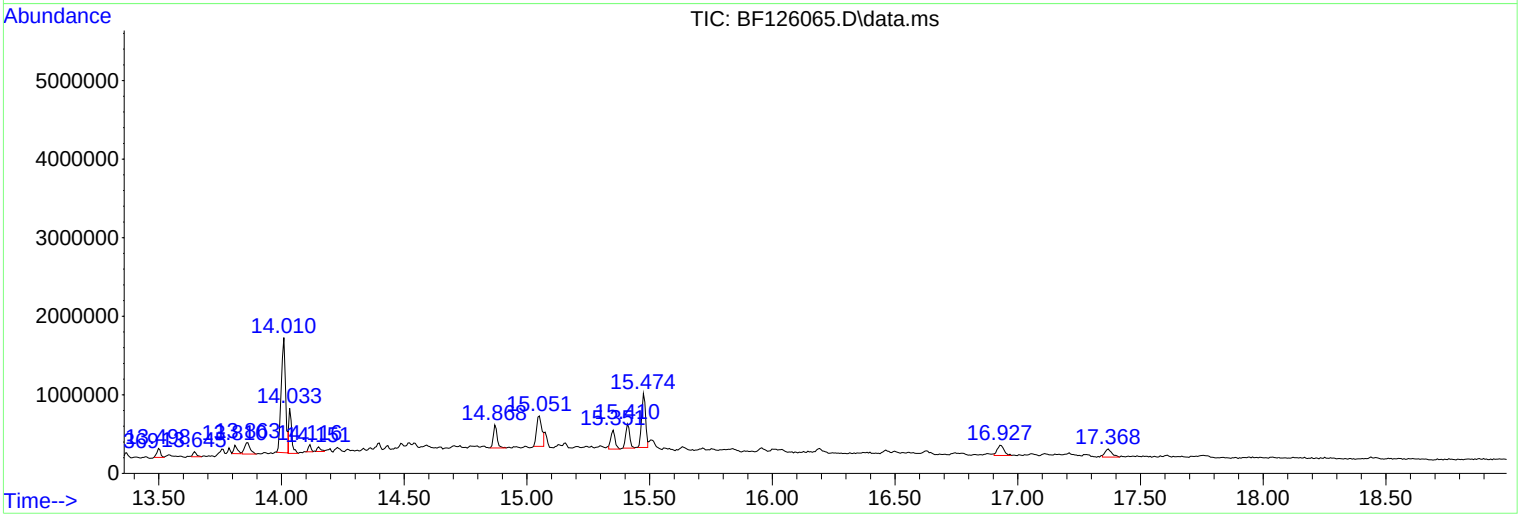
Instrument :
BNA_F
ClientSampleId :
WC-2-KS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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\BF110821\
Data File : BF126065.D
Acq On : 8 Nov 2021 15:04
Operator : JU/CG
Sample : M4472-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-KS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

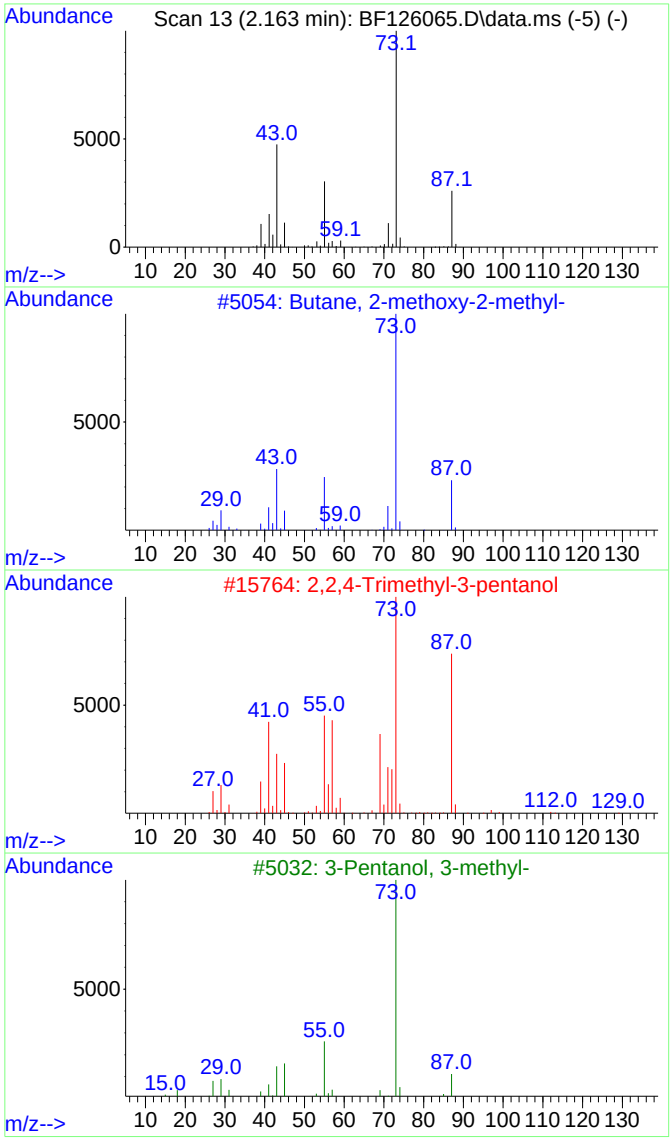
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

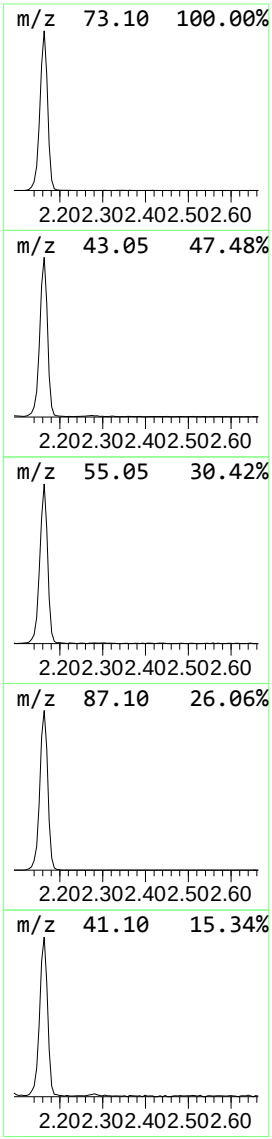
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	32.71 ng	1891990	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126065.D
Acq On : 8 Nov 2021 15:04
Operator : JU/CG
Sample : M4472-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-KS

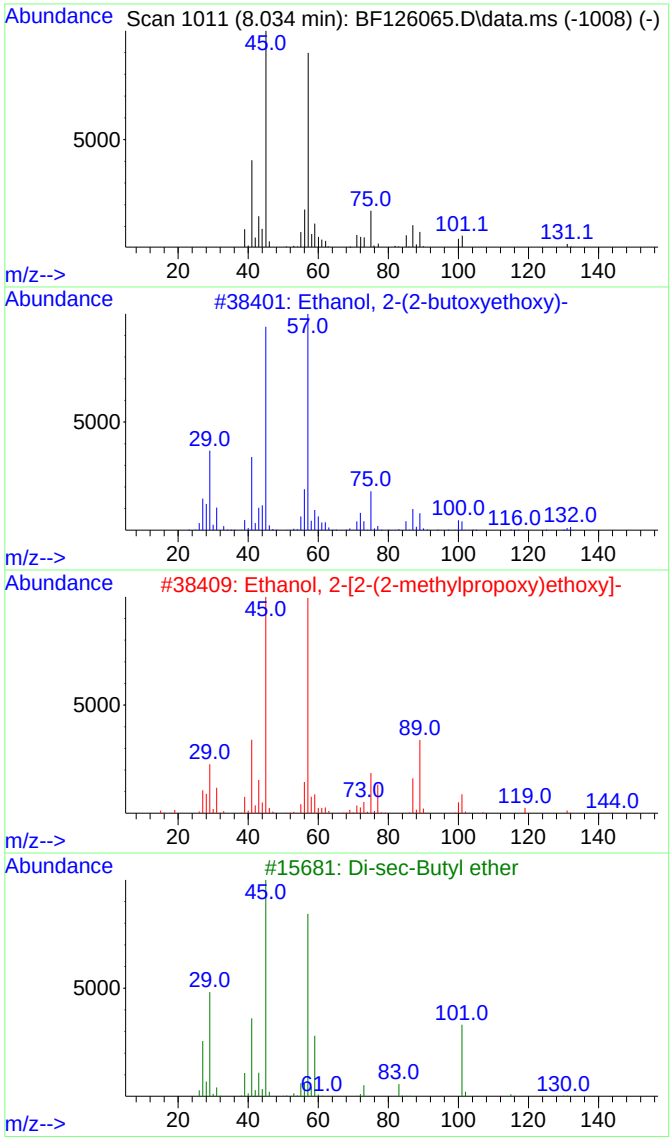
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

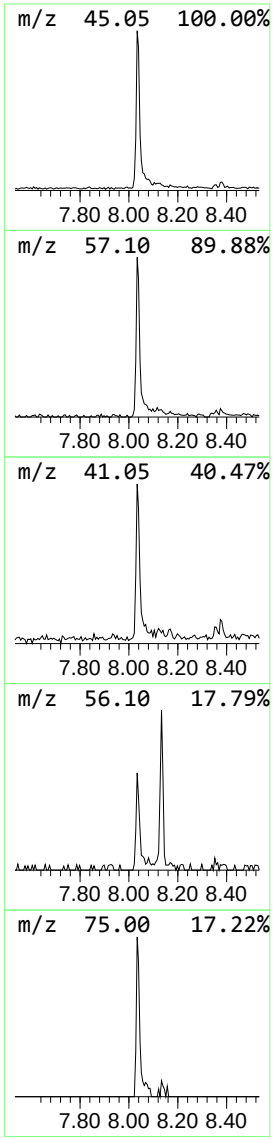
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	2.77 ng	193130	Naphthalene-d8	8.134

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50
5	3,6,9,12-Tetraoxatetradeca-1,13-...	202	C10H18O4	000765-12-8	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126065.D
Acq On : 8 Nov 2021 15:04
Operator : JU/CG
Sample : M4472-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-KS

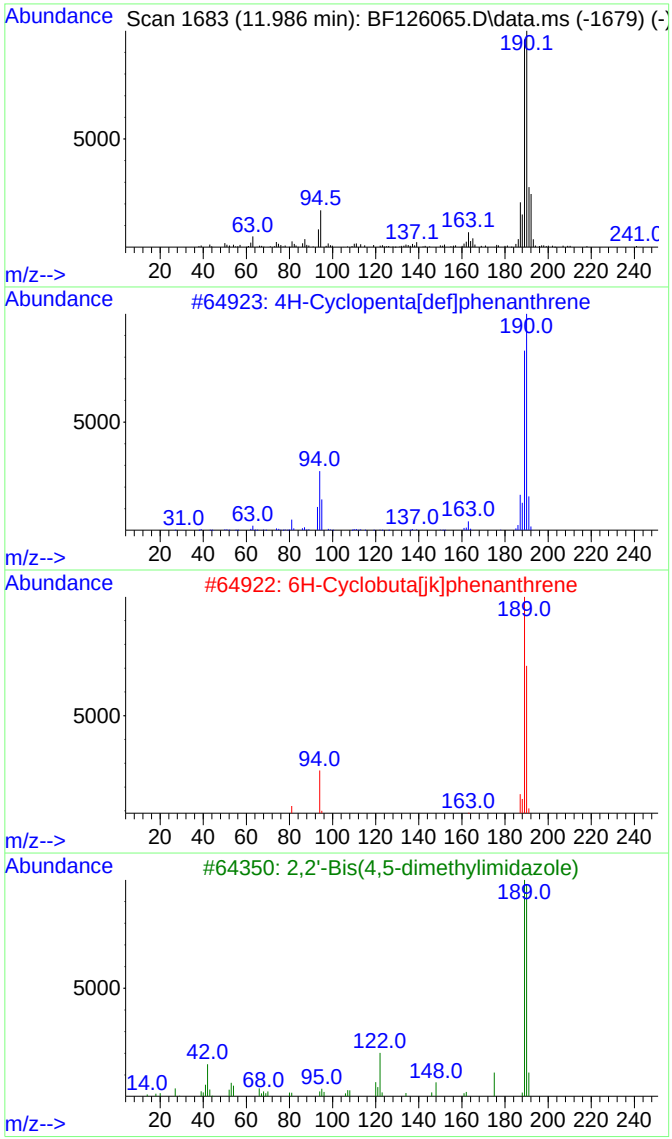
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

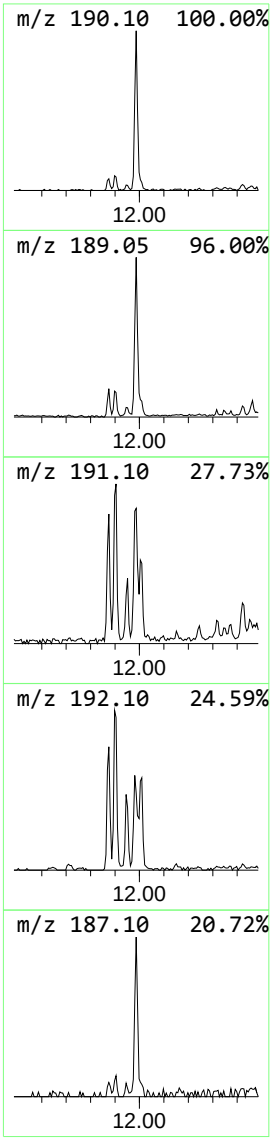
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	3.67 ng	234440	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	35
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126065.D
Acq On : 8 Nov 2021 15:04
Operator : JU/CG
Sample : M4472-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-KS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

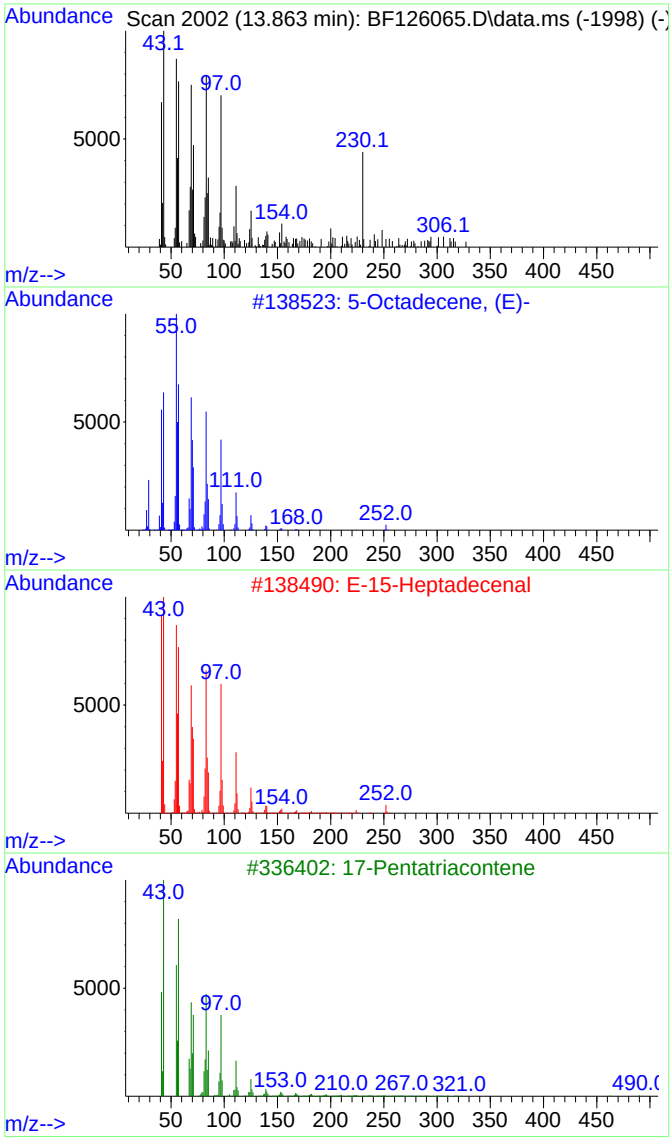
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

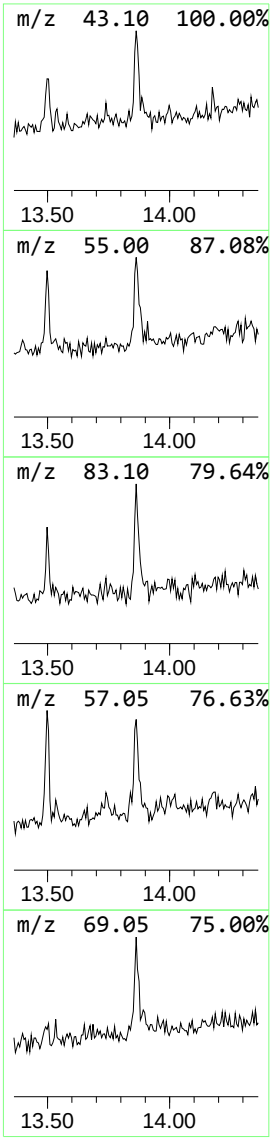
****

Peak Number 4 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	2.49 ng	230394	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	89
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	83
3	17-Pentatriacontene	491	C35H70	006971-40-0	80
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	80
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	78





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Data File : BF126065.D
Acq On : 8 Nov 2021 15:04
Operator : JU/CG
Sample : M4472-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-KS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

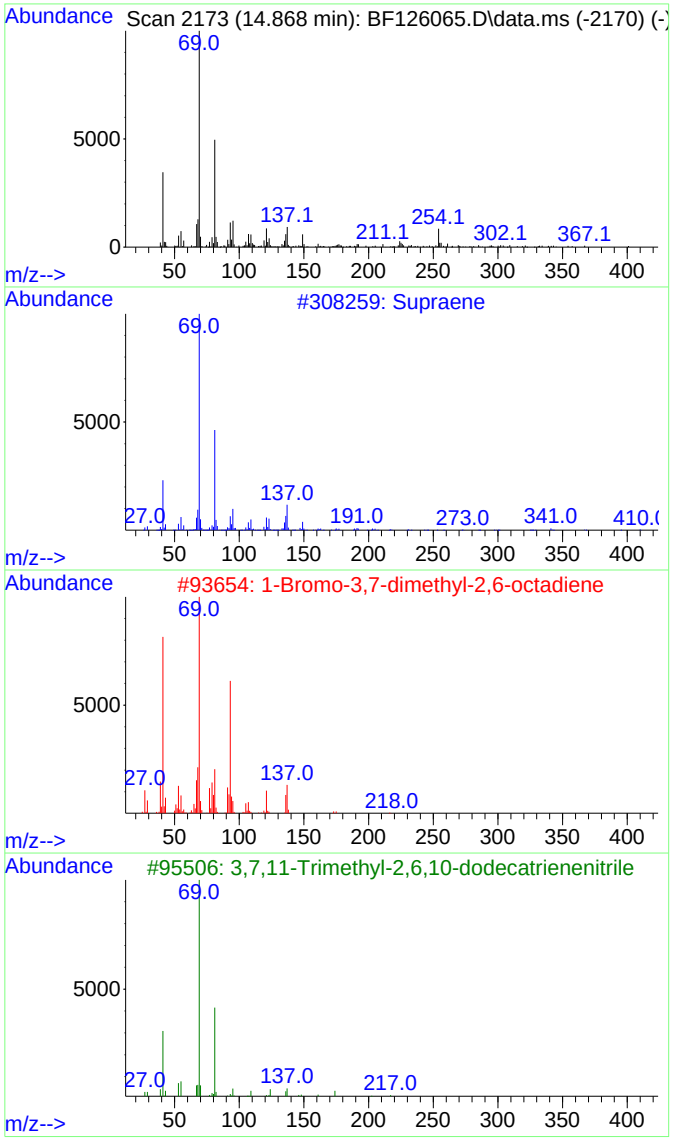
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

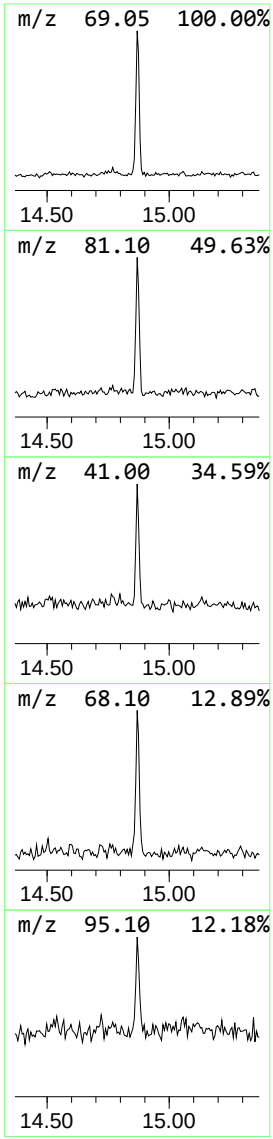
****

Peak Number 5 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	7.97 ng	311294	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	1-Bromo-3,7-dimethyl-2,6-octadiene	216	C10H17Br	035719-26-7	64
3	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110821\
Data File : BF126065.D
Acq On : 8 Nov 2021 15:04
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Sample : M4472-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2-KS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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
Butane, 2-metho...	2.163	32.7	ng	1891990	1	6.851	1156710	20.0
Ethanol, 2-(2-b...	8.034	2.8	ng	193130	2	8.134	1393540	20.0
4H-Cyclopenta[d...	11.986	3.7	ng	234440	4	11.369	1278180	20.0
5-Octadecene, (E)-	13.863	2.5	ng	230394	5	14.010	1852240	20.0
Supraene	14.868	8.0	ng	311294	6	15.474	781419	20.0