LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121947.D
Acq On : 13 Oct 2020 19:50
Operator : JU/CG
Sample : L4369-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-2

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: BF121947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.940	483	485	489	rBV	12559	14860	1.42%	0.126%
2	5.363	553	557	572	rBV	751395	916592	87.88%	7.781%
3	6.010	664	667	671	rBV	73504	66992	6.42%	0.569%
4	6.181	694	696	699	rBV	20703	16541	1.59%	0.140%
5	6.387	727	731	738	rBV	831171	892759	85.60%	7.578%
6	6.440	738	740	751	rVB	38238	46487	4.46%	0.395%
7	6.739	788	791	800	rBV	699687	658437	63.13%	5.589%
8	7.304	884	887	900	rBV	617193	615943	59.06%	5.229%
9	8.028	1006	1010	1027	rBV	925940	852748	81.76%	7.239%
10	9.098	1188	1192	1202	rBV	1255936	1042970	100.00%	8.854%
11	9.498	1256	1260	1268	rBV	86315	79783	7.65%	0.677%
12	9.775	1304	1307	1323	rVB	1017981	926713	88.85%	7.867%
13	10.569	1438	1442	1450	rBV	573755	592448	56.80%	5.029%
14	11.033	1518	1521	1525	rVB	17286	14762	1.42%	0.125%
15	11.263	1556	1560	1563	rBV	1051818	888413	85.18%	7.542%
16	11.286	1563	1564	1567	rVB	41385	22941	2.20%	0.195%
17	11.427	1584	1588	1592	rVB	12771	13220	1.27%	0.112%
18	11.627	1617	1622	1625	rBV6	7907	12485	1.20%	0.106%
19	11.763	1641	1645	1647	rBV3	15738	17272	1.66%	0.147%
20	11.792	1647	1650	1656	rVB6	14889	19795	1.90%	0.168%
21	11.874	1661	1664	1667	rBV4	11974	13348	1.28%	0.113%
22	12.139	1707	1709	1712	rVB4	19528	15647	1.50%	0.133%
23	12.227	1722	1724	1728	rBV3	21022	20816	2.00%	0.177%
24	12.298	1733	1736	1741	rBV4	71622	87037	8.35%	0.739%
25	12.474	1763	1766	1772	rVB	86404	75049	7.20%	0.637%
26	12.563	1778	1781	1785	rBV2	26807	34838	3.34%	0.296%
27	12.604	1786	1788	1794	rVV3	24108	45235	4.34%	0.384%
28	12.704	1800	1805	1810	rBV	80690	91202	8.74%	0.774%
29	12.845	1825	1829	1832	rBV	1079241	986133	94.55%	8.371%
30	13.080	1866	1869	1874	rBV4	22897	37606	3.61%	0.319%
31	13.245	1892	1897	1901	rBV6	31134	54814	5.26%	0.465%
32	13.321	1907	1910	1911	rBV	33007	32993	3.16%	0.280%
33	13.345	1911	1914	1917	rVB	353781	292270	28.02%	2.481%
34	13.698	1972	1974	1977	rBV	72702	65862	6.31%	0.559%
35	13.763	1982	1985	1992	rVB4	81369	144491	13.85%	1.227%
36	13.904	2005	2009	2012	rBV	935176	915811	87.81%	7.774%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121947.D
Acq On : 13 Oct 2020 19:50
Operator : JU/CG
Sample : L4369-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-2

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	14.027	2028	2030	2033	rVB	48256	37468	3.59%	0.318%
38	14.063	2034	2036	2039	rVB	68546	59850	5.74%	0.508%
39	14.098	2039	2042	2043	rBV2	34552	38379	3.68%	0.326%
40	14.221	2060	2063	2069	rBV2	69544	94079	9.02%	0.799%
41	15.339	2248	2253	2264	rBV	728056	925164	88.70%	7.854%

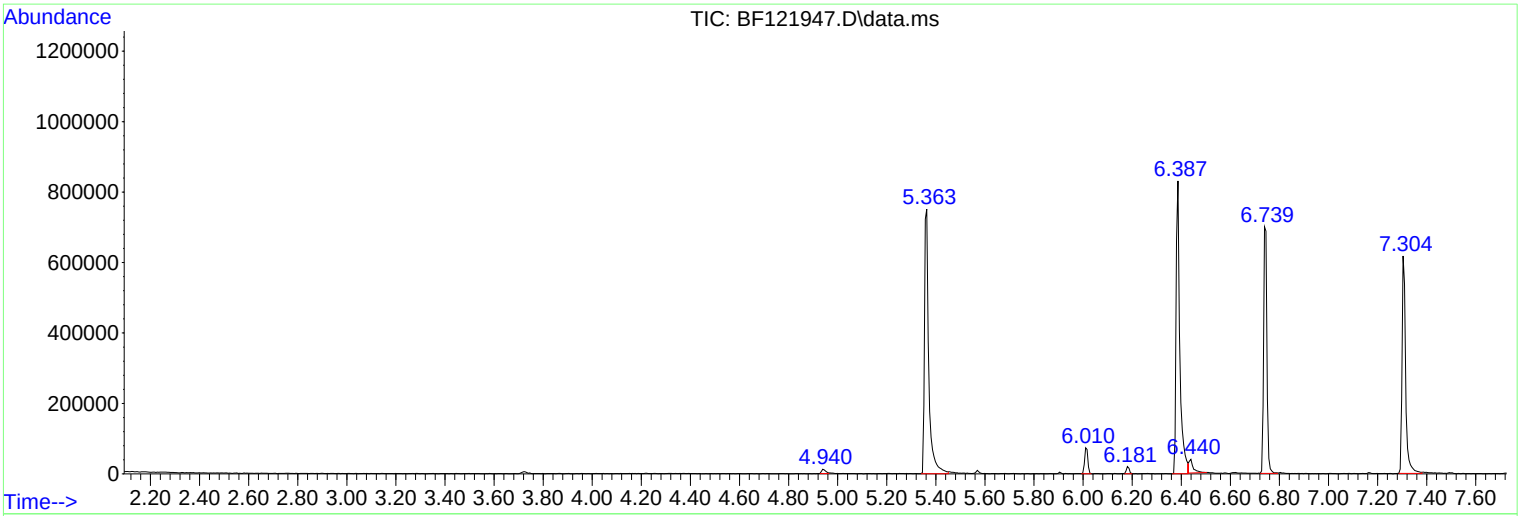
Sum of corrected areas: 11780253

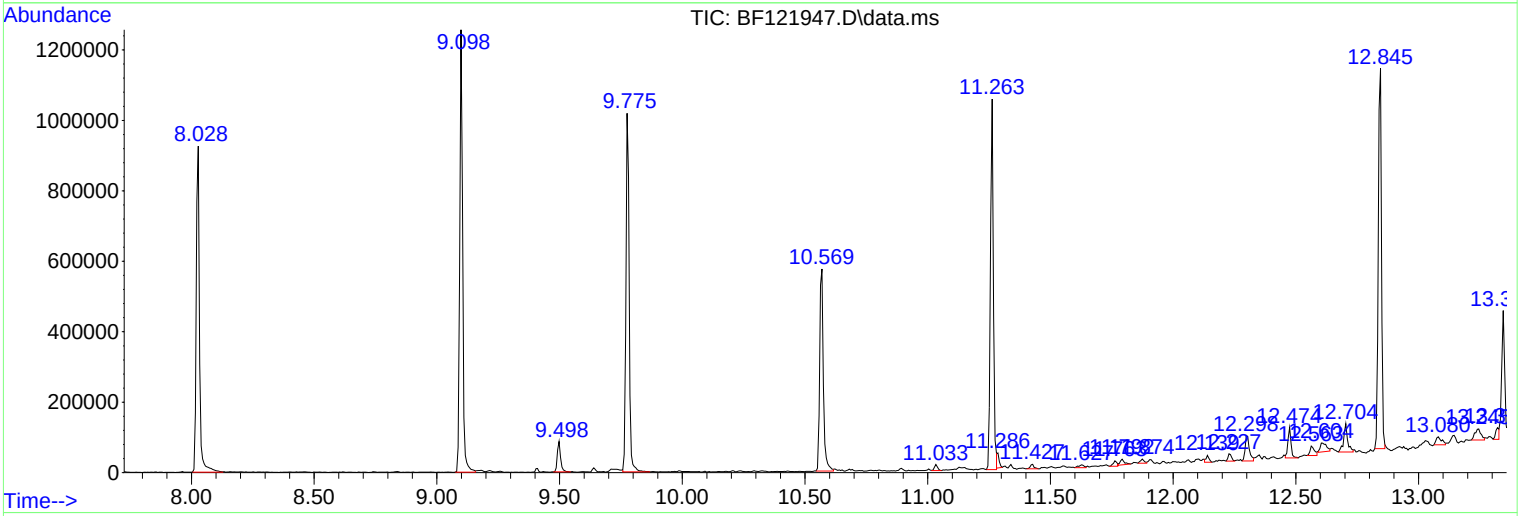
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121947.D
Acq On : 13 Oct 2020 19:50
Operator : JU/CG
Sample : L4369-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

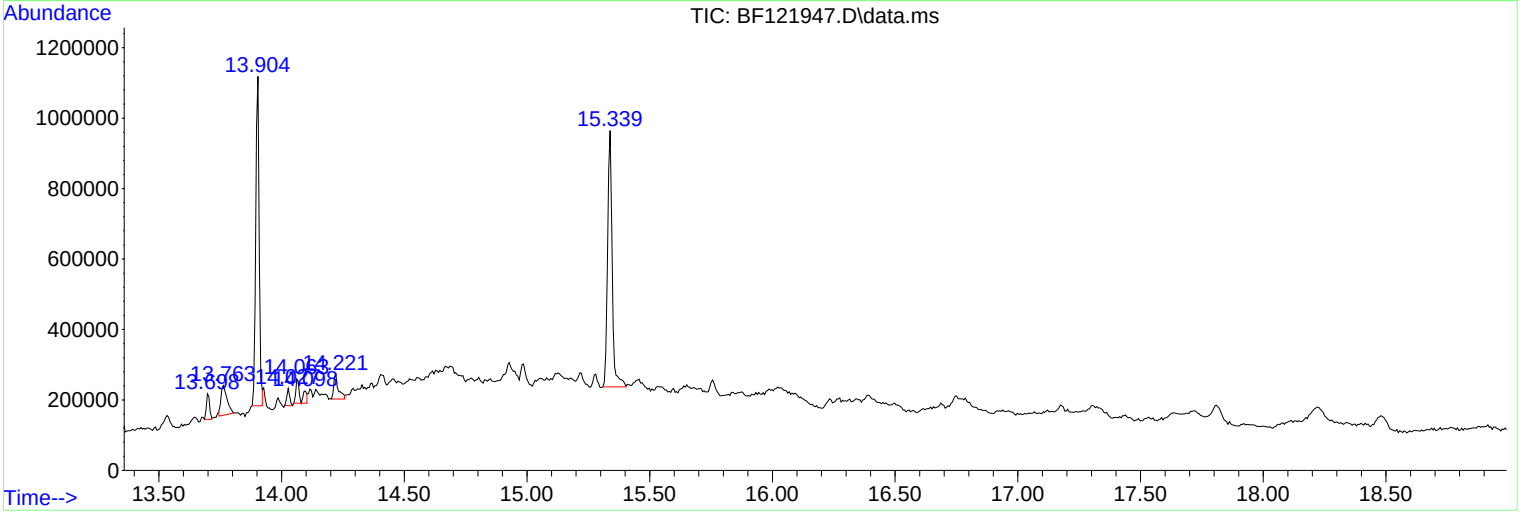
Instrument :
BNA_F
ClientSampleId :
HD-2

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\BF101320\
Data File : BF121947.D
Acq On : 13 Oct 2020 19:50
Operator : JU/CG
Sample : L4369-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-2

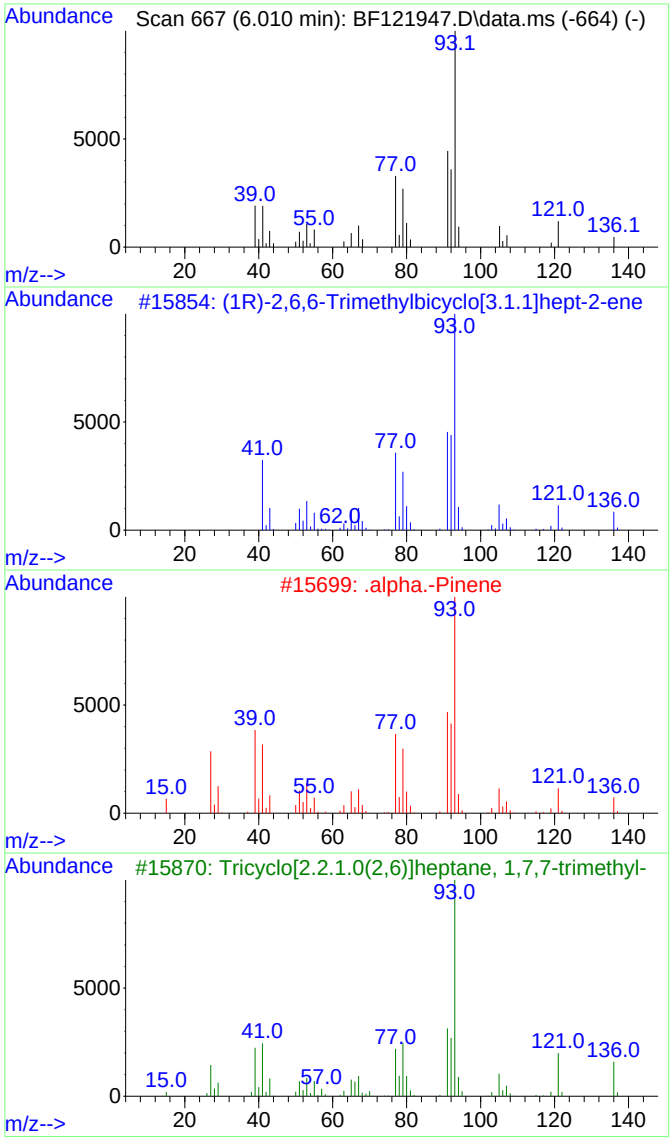
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

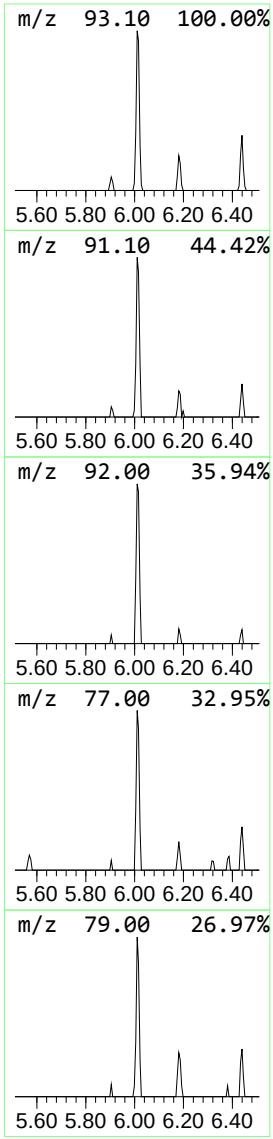
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.010	2.03 ng	66992	1,4-Dichlorobenzene-d4	6.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	96
2	.alpha.-Pinene	136	C10H16	000080-56-8	94
3	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	91
5	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121947.D
Acq On : 13 Oct 2020 19:50
Operator : JU/CG
Sample : L4369-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-2

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

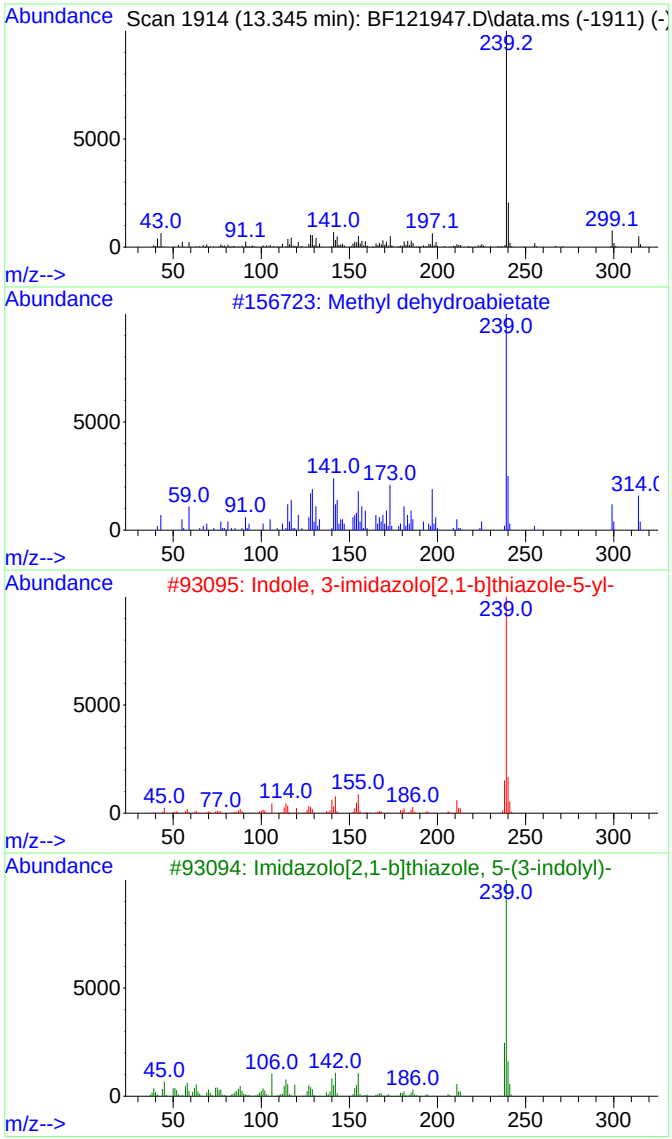
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

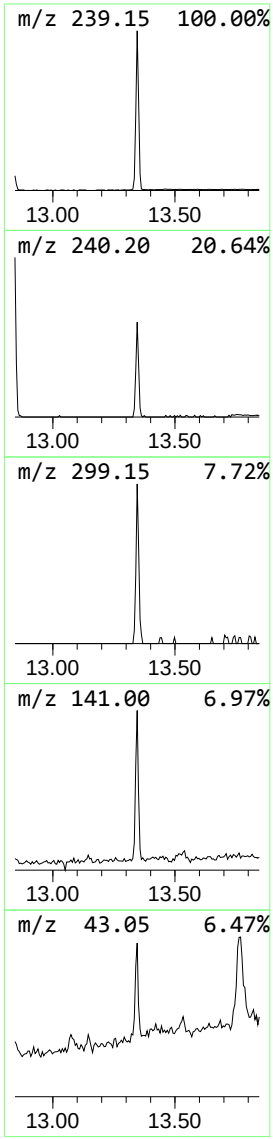
****

Peak Number 2 Methyl dehydroabietate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.345	6.38 ng	292270	Chrysene-d12	13.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl dehydroabietate	314	C21H30O2	001235-74-1	74
2	Indole, 3-imidazolo[2,1-b]thiazo...	239	C13H9N3S	292855-05-1	59
3	Imidazolo[2,1-b]thiazole, 5-(3-i...	239	C13H9N3S	327097-37-0	59
4	5-Nitro-3-phenyl-1H-indazole	239	C13H9N3O2	293758-67-5	45
5	9,10-Anthracenedione, 1-amino-4-...	239	C14H9NO3	000116-85-8	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121947.D
Acq On : 13 Oct 2020 19:50
Operator : JU/CG
Sample : L4369-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-2

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

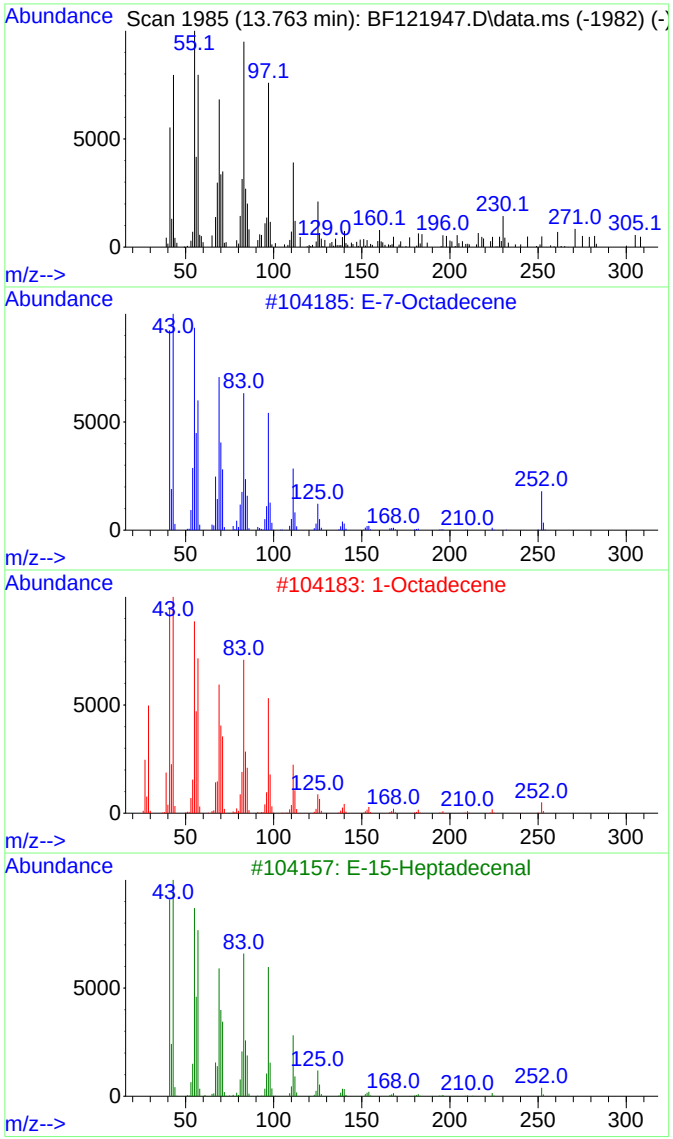
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

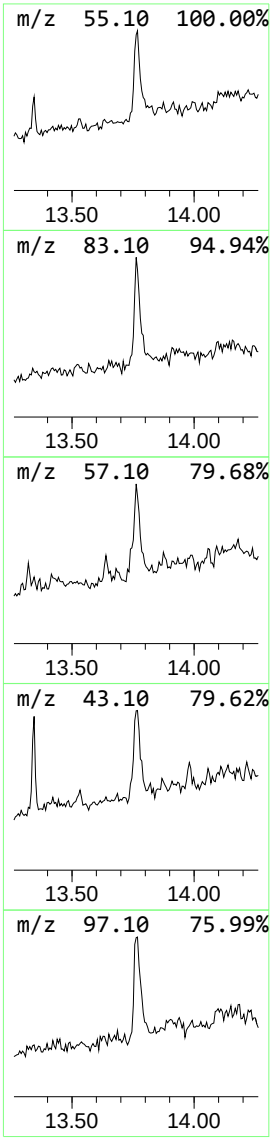
****

Peak Number 3 E-7-Octadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.763	3.16 ng	144491	Chrysene-d12	13.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-7-Octadecene	252	C18H36	1000130-92-0	93
2	1-Octadecene	252	C18H36	000112-88-9	90
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	89
4	Cyclohexadecane	224	C16H32	000295-65-8	87
5	1-Eicosanol	298	C20H42O	000629-96-9	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121947.D
Acq On : 13 Oct 2020 19:50
Operator : JU/CG
Sample : L4369-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-2

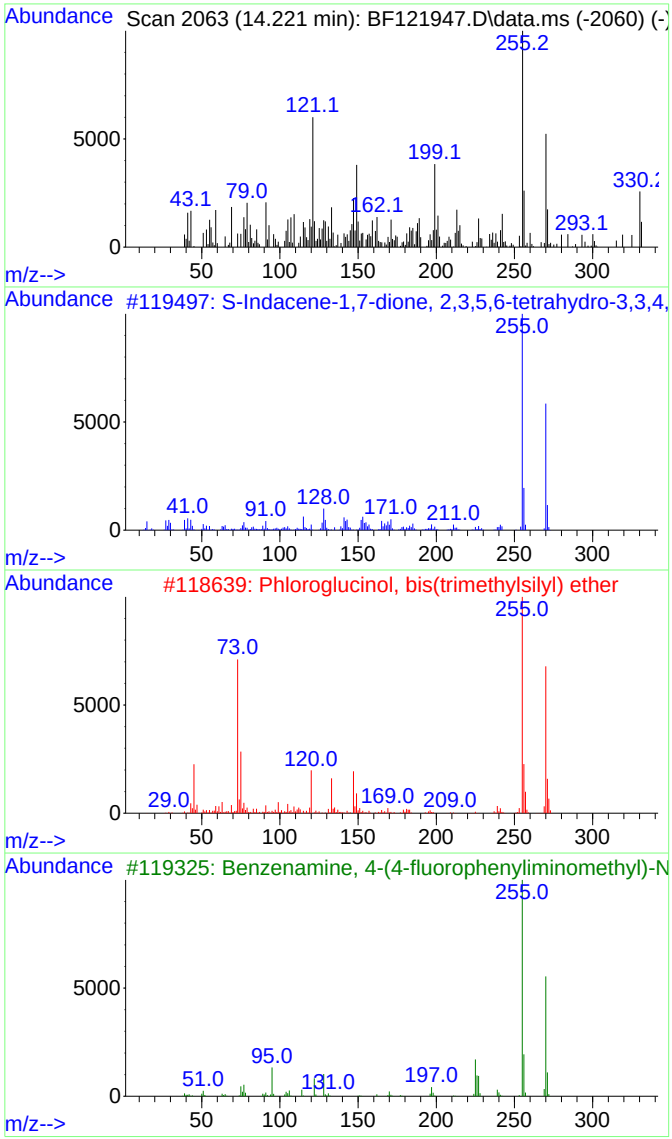
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

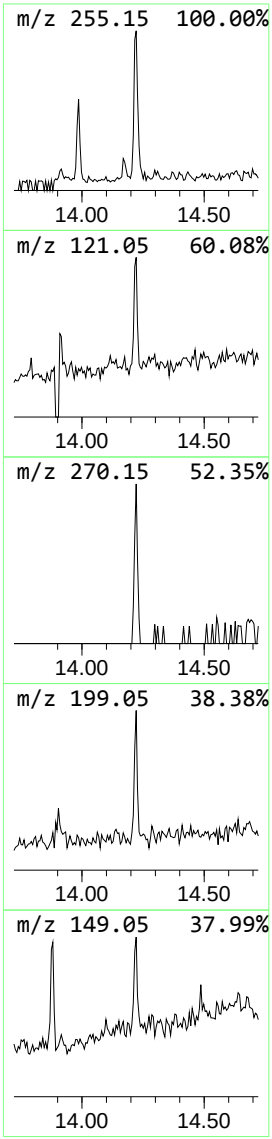
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 S-Indacene-1,7-dione, 2,3,5... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	2.05 ng	94079	Chrysene-d12	13.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Indacene-1,7-dione, 2,3,5,6-te...	270	C18H22O2	055591-16-7	64
2	Phloroglucinol, bis(trimethylsil...	270	C12H22O3Si2	1000352-45-8	46
3	Benzenamine, 4-(4-fluorophenylim...	270	C17H19FN2	1000260-40-0	45
4	1-[4-Acetyl-1-(4-amino-phenyl)-2...	270	C16H18N2O2	1000300-67-2	45
5	4H-Naphtho[1,2-b]pyran-4-one, 5,...	270	C16H14O4	032454-45-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101320\
Data File : BF121947.D
Acq On : 13 Oct 2020 19:50
Operator : JU/CG
Sample : L4369-04 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-2

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(1R)-2,6,6-Trim...	6.010	2.0	ng	66992	1	6.745	658437	20.0
Methyl dehydroa...	13.345	6.4	ng	292270	5	13.904	915811	20.0
E-7-Octadecene	13.763	3.2	ng	144491	5	13.904	915811	20.0
S-Indacene-1,7-...	14.221	2.0	ng	94079	5	13.904	915811	20.0