LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136425.D
Acq On : 06 Dec 2023 13:29
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12018

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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136425.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	496	500	506	rVB	60992	69267	3.34%	0.392%
2	5.228	530	534	542	rBV	59564	67770	3.27%	0.384%
3	5.428	564	568	571	rBV	1932750	1773720	85.45%	10.049%
4	6.081	675	679	682	rVB	577940	471947	22.74%	2.674%
5	6.246	701	707	711	rBV	54149	45273	2.18%	0.256%
6	6.428	733	738	741	rBV	1784685	1830211	88.18%	10.369%
7	6.498	747	750	753	rVB	236262	182432	8.79%	1.034%
8	6.634	767	773	776	rBV2	15834	26308	1.27%	0.149%
9	6.745	789	792	797	rVB	47343	36412	1.75%	0.206%
10	6.793	797	800	804	rBV	751462	611634	29.47%	3.465%
11	7.357	891	896	899	rBV	1339459	1244697	59.97%	7.052%
12	8.069	1013	1017	1021	rBV	900006	794041	38.26%	4.498%
13	9.151	1196	1201	1204	rBV	2605246	2075643	100.00%	11.759%
14	9.269	1218	1221	1226	rBV	36041	42204	2.03%	0.239%
15	9.486	1255	1258	1260	rVB2	32527	28366	1.37%	0.161%
16	9.828	1312	1316	1319	rBV	1060600	825598	39.78%	4.677%
17	10.616	1446	1450	1463	rVB	1104812	977573	47.10%	5.538%
18	11.316	1566	1569	1572	rBV	863177	738019	35.56%	4.181%
19	11.339	1572	1573	1577	rVV	172227	111171	5.36%	0.630%
20	11.392	1577	1582	1586	rVB	39678	38797	1.87%	0.220%
21	11.710	1631	1636	1637	rBV2	19500	26853	1.29%	0.152%
22	11.851	1657	1660	1665	rBV	166016	165902	7.99%	0.940%
23	11.933	1671	1674	1676	rBV	24604	25805	1.24%	0.146%
24	12.210	1717	1721	1724	rVB	39732	34299	1.65%	0.194%
25	12.457	1752	1763	1773	rBV5	152316	606344	29.21%	3.435%
26	12.533	1773	1776	1782	rVB	252568	247497	11.92%	1.402%
27	12.645	1792	1795	1800	rBV3	50447	58015	2.80%	0.329%
28	12.763	1809	1815	1818	rBV	185310	188812	9.10%	1.070%
29	12.916	1837	1841	1844	rVB	1344104	1239274	59.71%	7.021%
30	13.092	1864	1871	1875	rBV2	29492	52345	2.52%	0.297%
31	13.157	1879	1882	1885	rVB3	23739	29734	1.43%	0.168%
32	13.216	1890	1892	1897	rVB5	24457	33147	1.60%	0.188%
33	13.433	1926	1929	1931	rBV3	68883	62043	2.99%	0.351%
34	13.463	1931	1934	1936	rVB	43187	41894	2.02%	0.237%
35	13.522	1942	1944	1948	rVB4	35512	30563	1.47%	0.173%
36	13.827	1991	1996	2001	rVB2	46080	63647	3.07%	0.361%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136425.D
Acq On : 06 Dec 2023 13:29
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12018

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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.963	2013	2019	2023	rBV2	918228	1156988	55.74%	6.555%
38	13.992	2023	2024	2031	rVB	116060	103200	4.97%	0.585%
39	14.145	2048	2050	2053	rVB	31968	25180	1.21%	0.143%
40	14.192	2055	2058	2069	rBV5	123698	173898	8.38%	0.985%
41	14.451	2099	2102	2105	rVB2	55756	53495	2.58%	0.303%
42	14.763	2153	2155	2161	rVB	36139	41949	2.02%	0.238%
43	15.010	2193	2197	2201	rBV	100953	167679	8.08%	0.950%
44	15.110	2211	2214	2219	rVB3	44297	69332	3.34%	0.393%
45	15.316	2246	2249	2256	rVB	53944	81351	3.92%	0.461%
46	15.380	2256	2260	2267	rBV	80047	102934	4.96%	0.583%
47	15.445	2267	2271	2275	rBV	492975	607456	29.27%	3.441%
48	15.951	2353	2357	2365	rVB	31476	53673	2.59%	0.304%
49	16.939	2520	2525	2534	rVB3	32661	69031	3.33%	0.391%
50	17.392	2596	2602	2607	rBV3	23902	47996	2.31%	0.272%

Sum of corrected areas: 17651419

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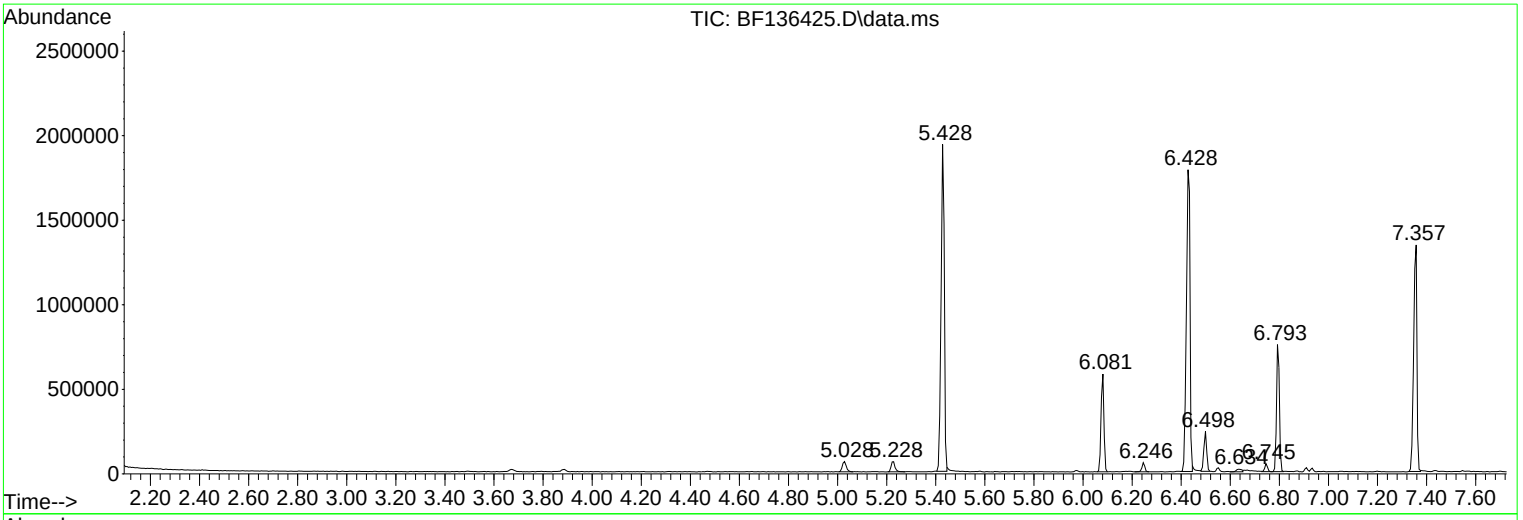
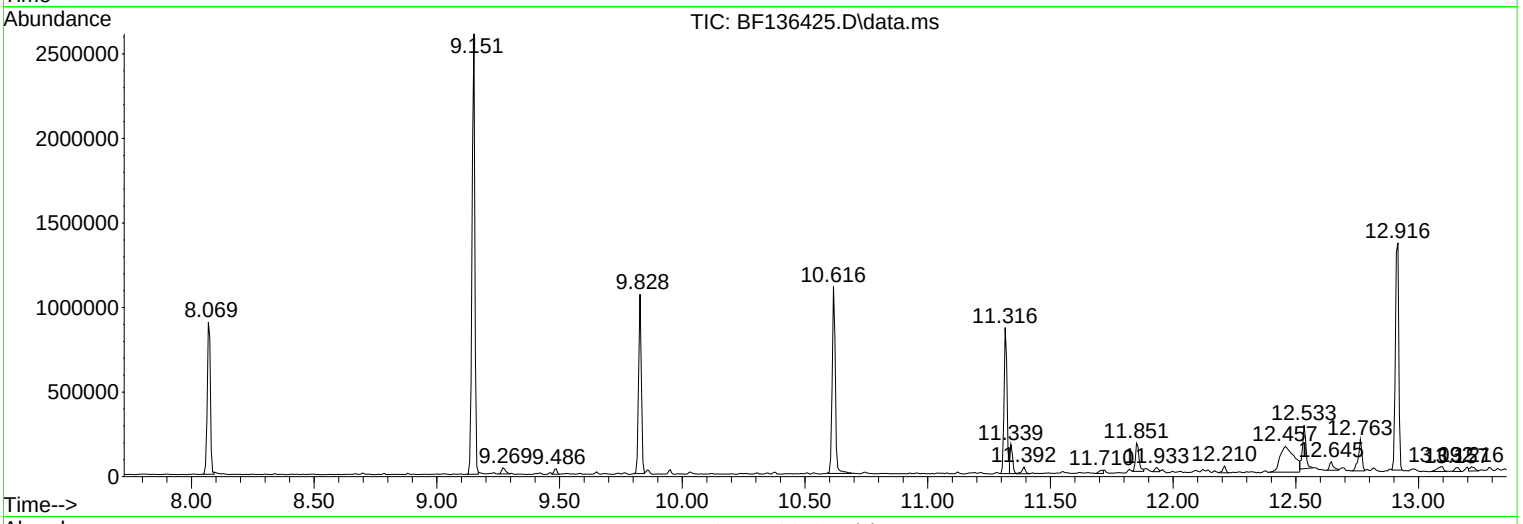
Misc :
ALS Vial : 8 Sample Multiplier: 1

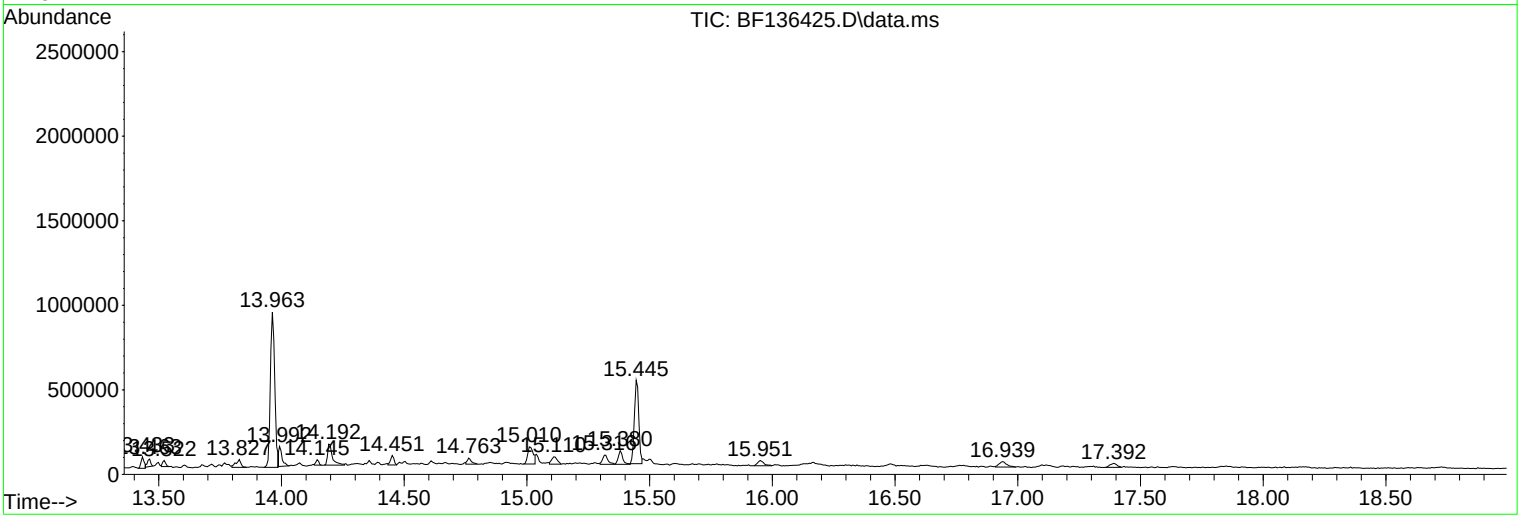
Instrument :
BNA_F
ClientSampleId :
72-12018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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\BF120623\
Data File : BF136425.D
Acq On : 06 Dec 2023 13:29
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
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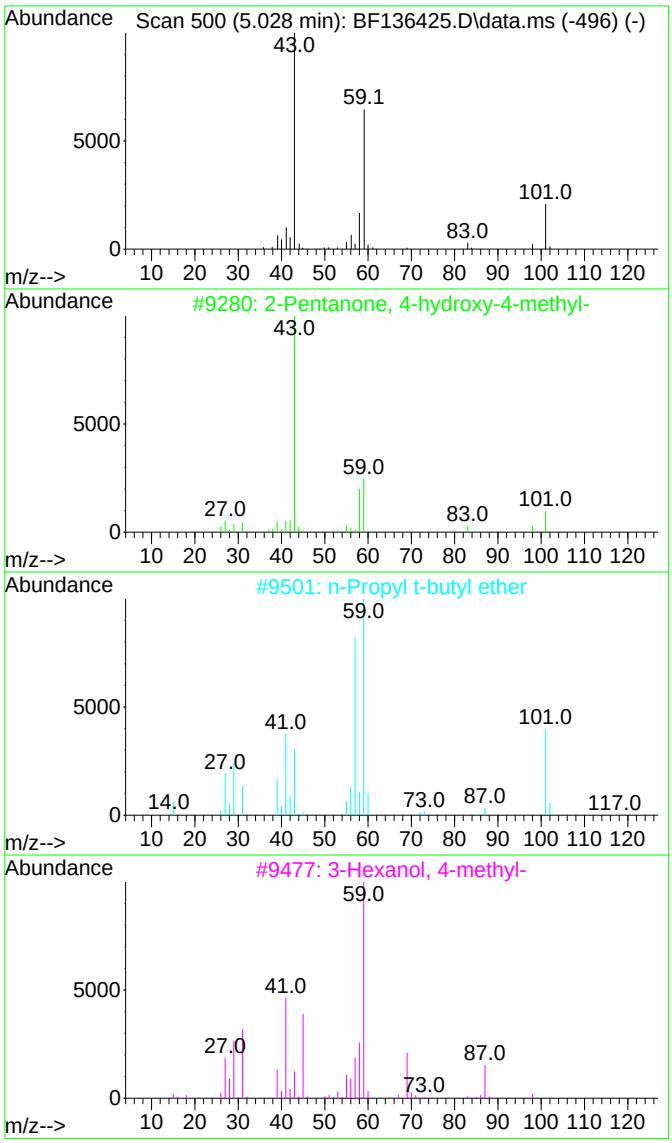
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

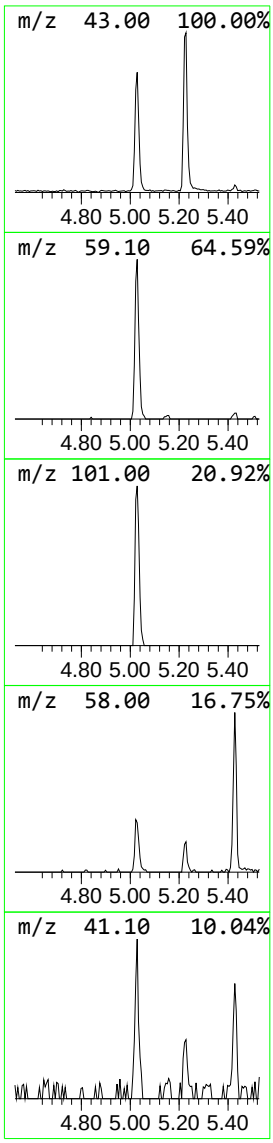
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	2.26 ng	69267	1,4-Dichlorobenzene-d4	6.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetone	58	C3H6O	000067-64-1	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136425.D
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Operator : CG\JU
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12018

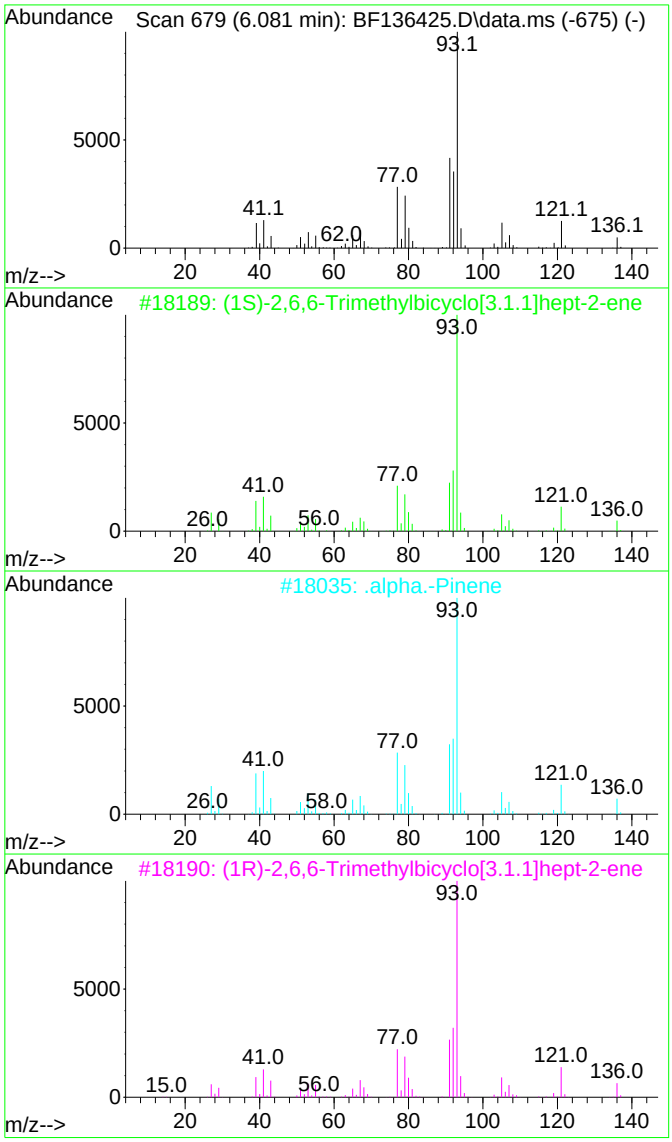
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

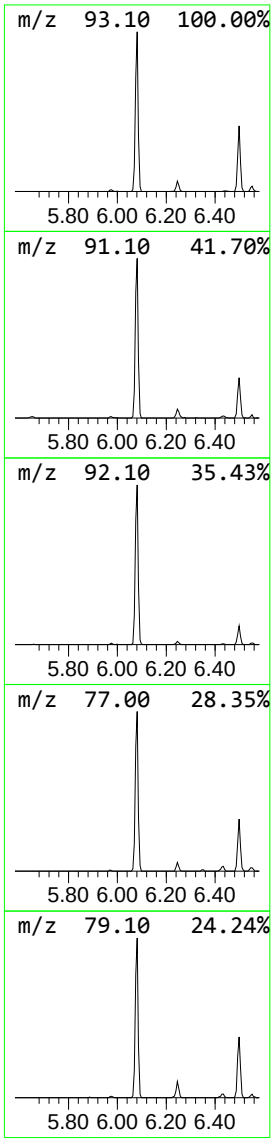
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (1S)-2,6,6-Trimethylbicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.081	15.43 ng	471947	1,4-Dichlorobenzene-d4	6.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	96
2	.alpha.-Pinene	136	C10H16	000080-56-8	95
3	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
4	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	91
5	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
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Acq On : 06 Dec 2023 13:29
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12018

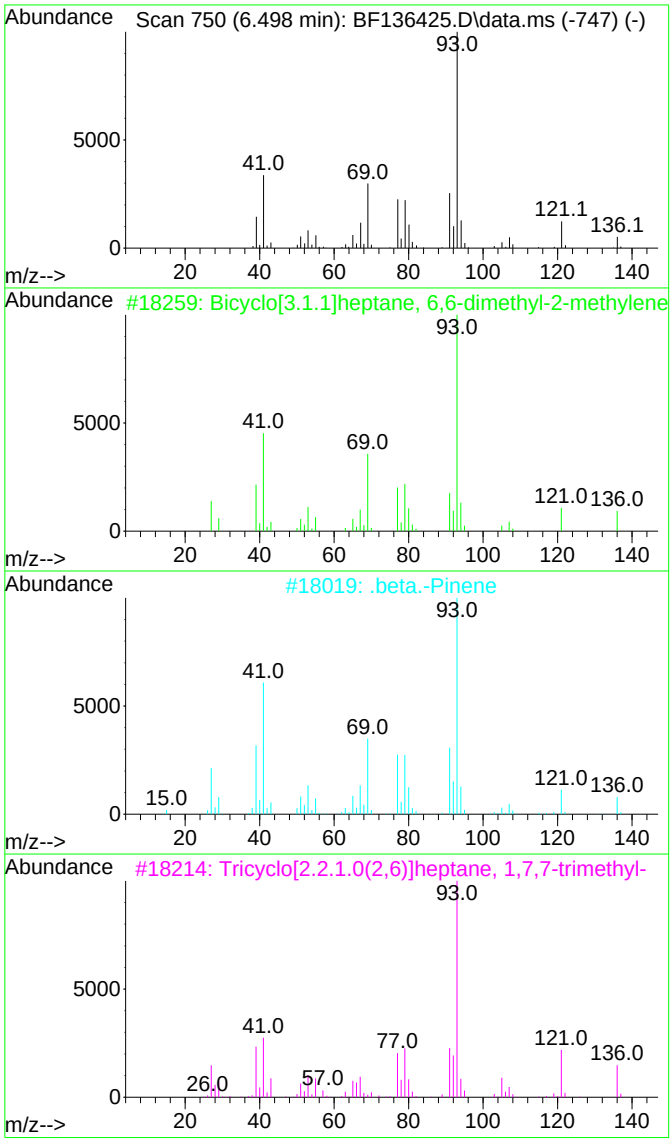
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

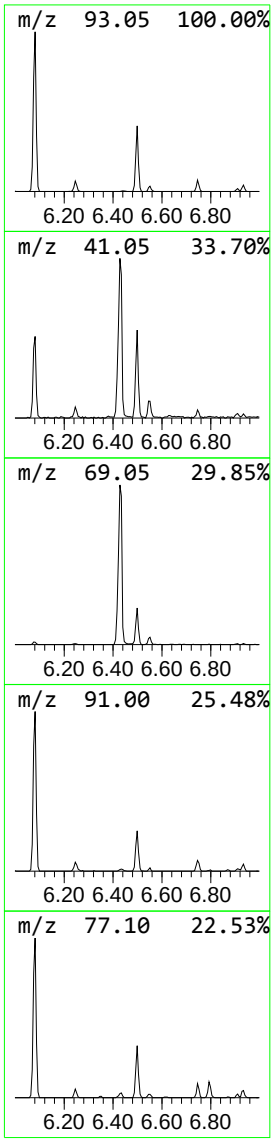
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Bicyclo[3.1.1]heptane, 6,6-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.498	5.97 ng	182432	1,4-Dichlorobenzene-d4	6.793

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	94
2	.beta.-Pinene	136	C10H16	000127-91-3	93
3	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4	Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	87
5	.beta.-Myrcene	136	C10H16	000123-35-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136425.D
Acq On : 06 Dec 2023 13:29
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

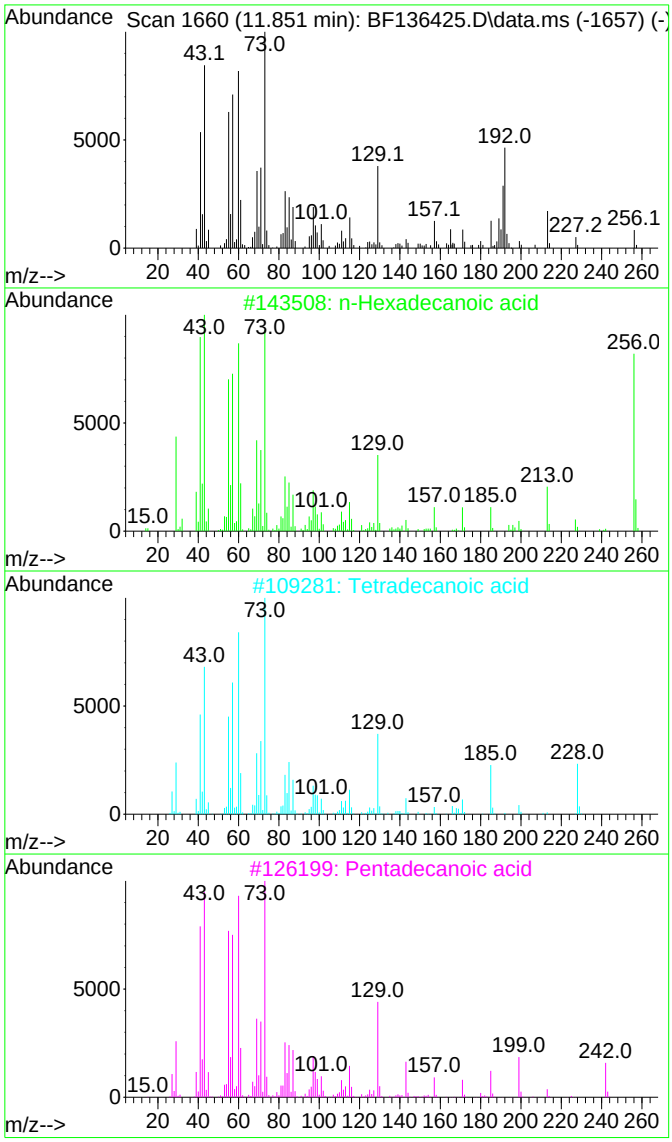
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

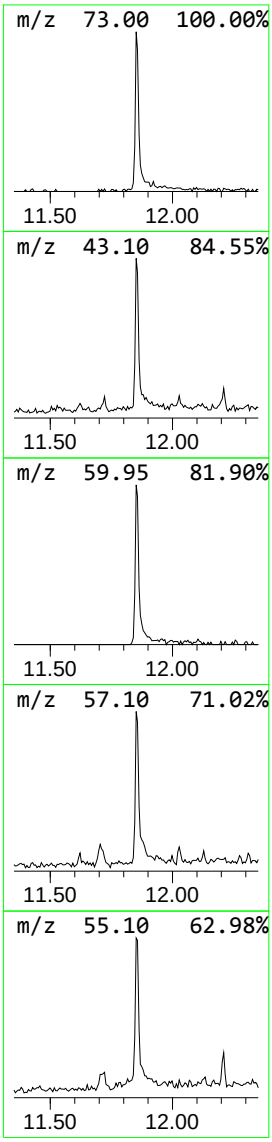
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	4.50 ng	165902	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136425.D
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

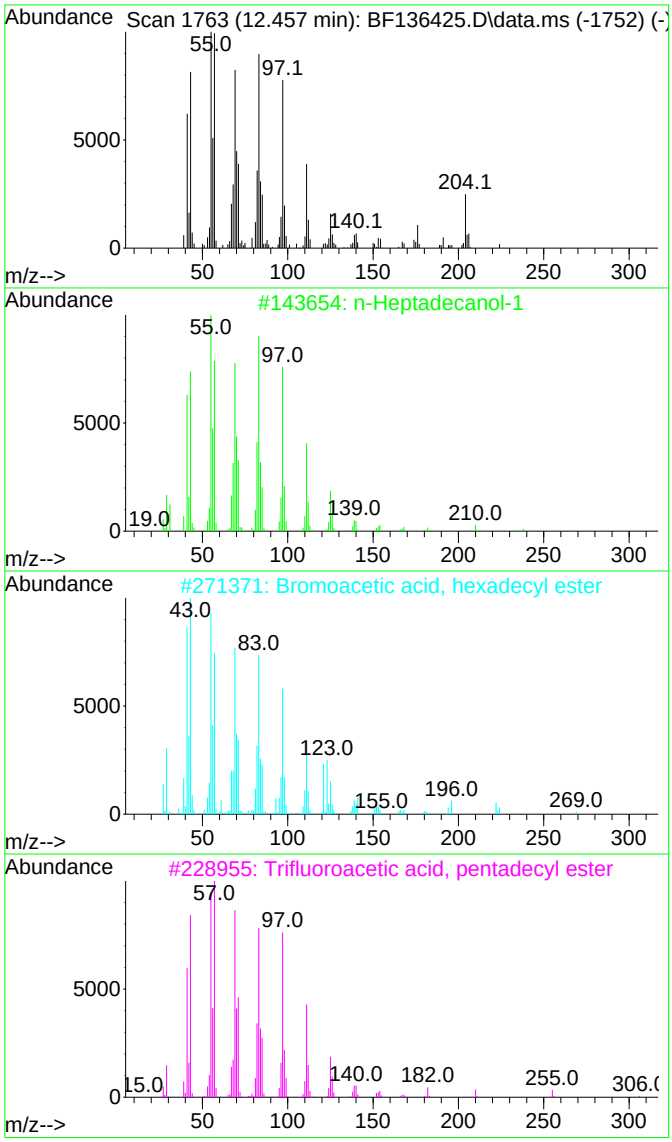
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

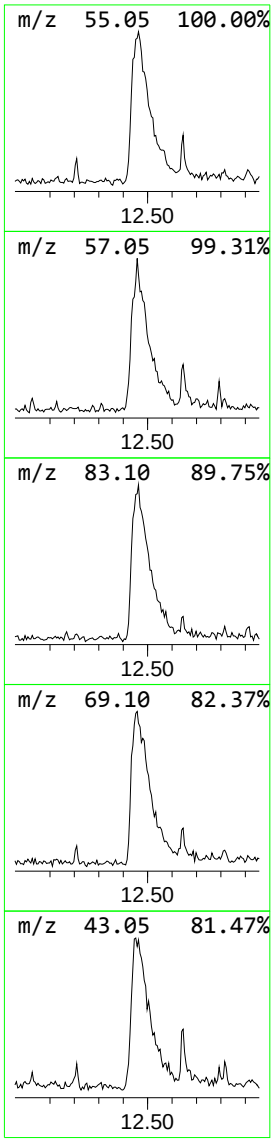
****

Peak Number 6 n-Heptadecanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	16.43 ng	606344	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	1-Octadecanol	270	C18H38O	000112-92-5	93
5	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136425.D
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Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

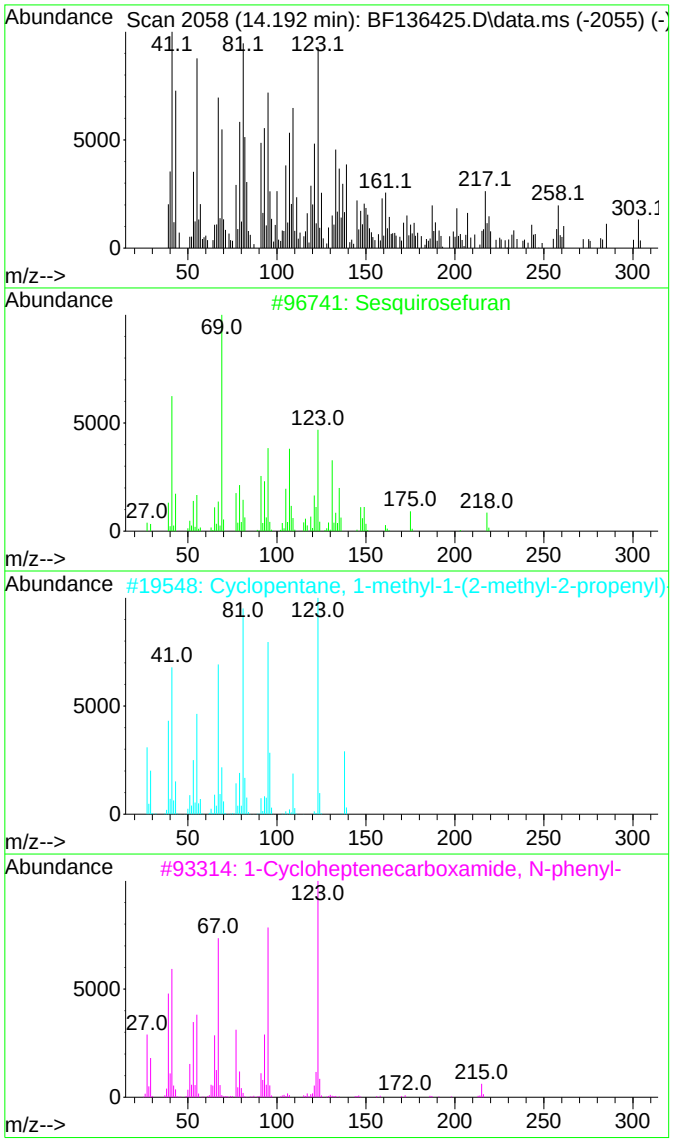
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

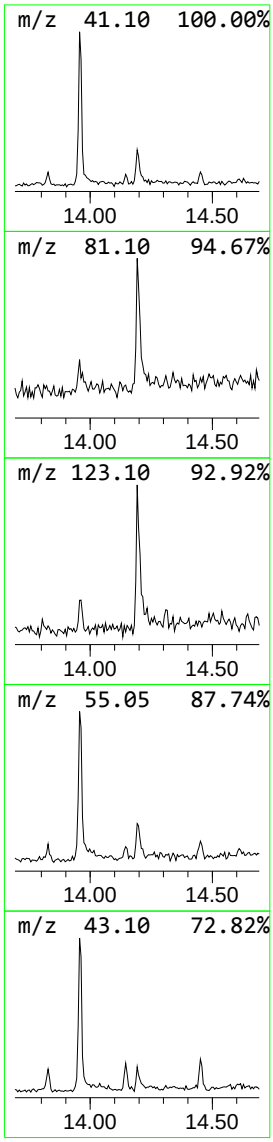
****

Peak Number 7 Sesquirosefuran Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	3.01 ng	173898	Chrysene-d12	13.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sesquirosefuran	218	C15H22O	039007-93-7	56
2	Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	50
3	1-Cycloheptenecarboxamide, N-phe...	215	C14H17NO	1000158-85-5	47
4	(4E,8E,13E)-1-(2-Hydroxyethyl)-1...	276	C19H32O	1000426-96-0	46
5	2-Cyclohexene-1-methanol, 2,6,6-...	154	C10H18O	006627-74-3	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136425.D
Acq On : 06 Dec 2023 13:29
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

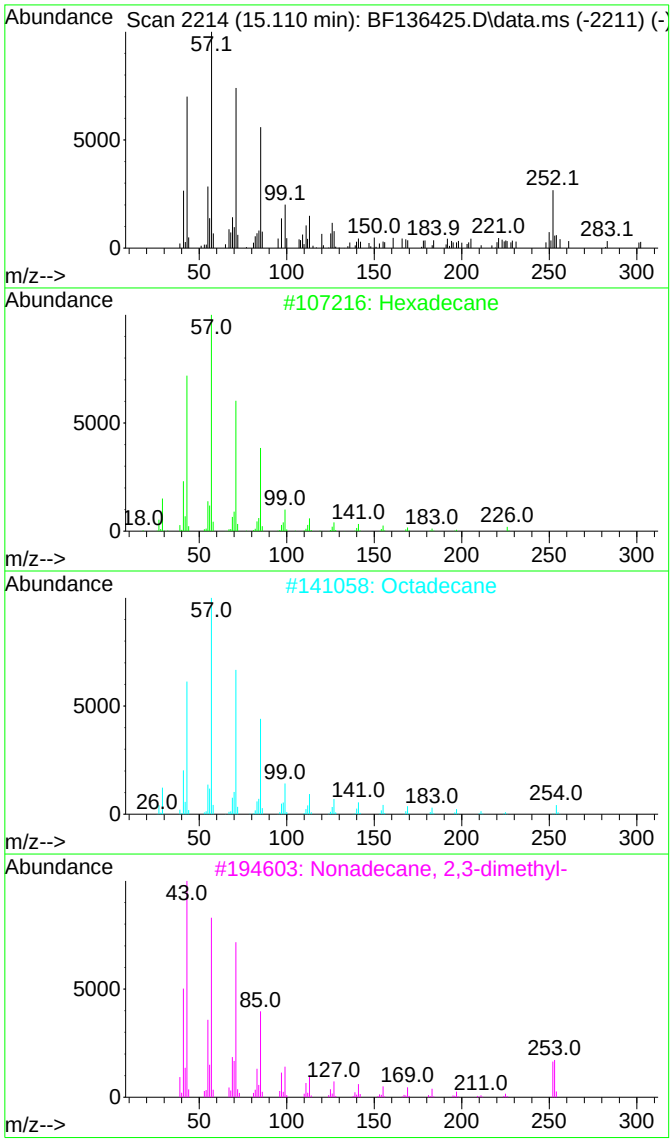
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

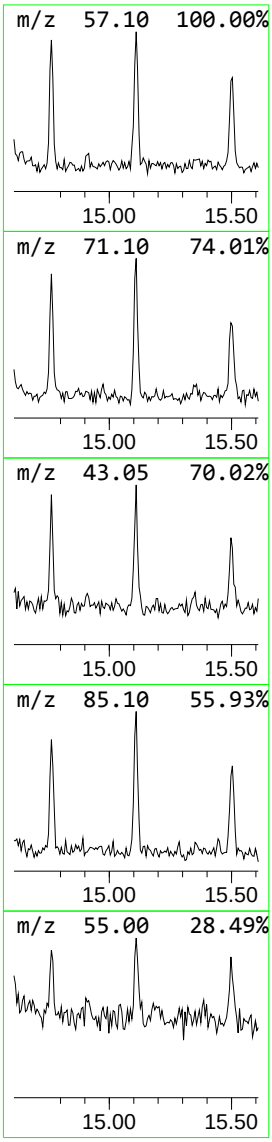
****

Peak Number 8 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	2.28 ng	69332	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Octadecane	254	C18H38	000593-45-3	86
3	Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	72
4	Tetradecane	198	C14H30	000629-59-4	64
5	Heneicosane	296	C21H44	000629-94-7	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136425.D
Acq On : 06 Dec 2023 13:29
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

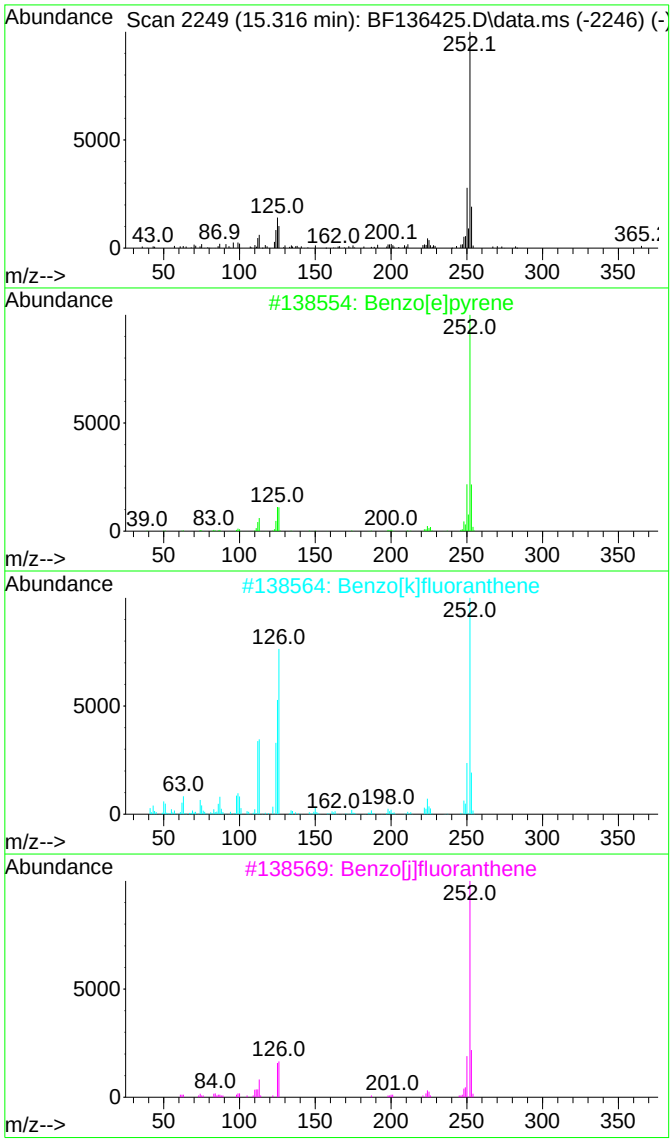
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

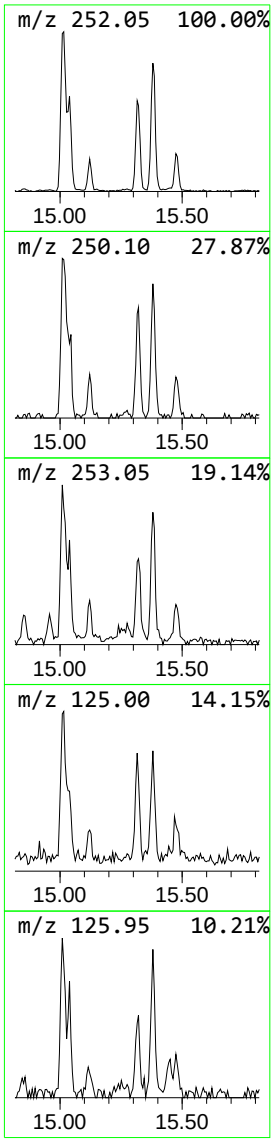
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.316	2.68 ng	81351	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Perylene	252	C20H12	000198-55-0	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120623\
Data File : BF136425.D
Acq On : 06 Dec 2023 13:29
Operator : CG\JU
Sample : 05420-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12018

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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
2-Pentanone, 4-...	5.028	2.3	ng	69267	1	6.793	611634	20.0
(1S)-2,6,6-Trim...	6.081	15.4	ng	471947	1	6.793	611634	20.0
Bicyclo[3.1.1]h...	6.498	6.0	ng	182432	1	6.793	611634	20.0
n-Hexadecanoic ...	11.851	4.5	ng	165902	4	11.316	738019	20.0
n-Heptadecanol-1	12.457	16.4	ng	606344	4	11.316	738019	20.0
Sesquirosefuran	14.192	3.0	ng	173898	5	13.969	1156990	20.0
Hexadecane	15.110	2.3	ng	69332	6	15.445	607456	20.0
Benzo[e]pyrene	15.316	2.7	ng	81351	6	15.445	607456	20.0