LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11944

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.134	480	484	490	rVB	82343	100462	2.98%	0.384%
2	5.528	546	551	554	rBV	2776852	2729792	80.98%	10.438%
3	6.528	716	721	724	rBV	2778102	2932902	87.00%	11.215%
4	6.898	781	784	788	rBV	749292	608343	18.05%	2.326%
5	7.463	875	880	883	rBV	2020149	1992663	59.11%	7.620%
6	8.075	981	984	989	rBV	43615	47547	1.41%	0.182%
7	8.181	999	1002	1005	rBV	956662	811386	24.07%	3.103%
8	9.263	1181	1186	1189	rBV	3675961	3371024	100.00%	12.890%
9	9.522	1226	1230	1234	rBV2	32641	43384	1.29%	0.166%
10	9.598	1239	1243	1245	rBV	39702	42089	1.25%	0.161%
11	9.939	1298	1301	1304	rVV	983274	845418	25.08%	3.233%
12	9.975	1304	1307	1310	rVB	109752	86816	2.58%	0.332%
13	10.145	1330	1336	1339	rVB	120172	106916	3.17%	0.409%
14	10.486	1388	1394	1399	rVB	204197	189862	5.63%	0.726%
15	10.733	1432	1436	1439	rBV	2691140	2288353	67.88%	8.750%
16	10.857	1455	1457	1463	rVB	62762	61952	1.84%	0.237%
17	11.039	1482	1488	1490	rBV3	47958	62605	1.86%	0.239%
18	11.233	1517	1521	1524	rVB	40714	36816	1.09%	0.141%
19	11.280	1525	1529	1532	rVV2	42986	50430	1.50%	0.193%
20	11.327	1532	1537	1541	rVB	53258	58884	1.75%	0.225%
21	11.433	1551	1555	1557	rBV	1013531	880236	26.11%	3.366%
22	11.457	1557	1559	1562	rVV	838351	615799	18.27%	2.355%
23	11.504	1562	1567	1570	rVB	155824	146611	4.35%	0.561%
24	11.663	1590	1594	1600	rBV	53113	61224	1.82%	0.234%
25	11.945	1635	1642	1643	rBV2	101039	152753	4.53%	0.584%
26	11.963	1643	1645	1647	rVB	117952	88205	2.62%	0.337%
27	12.010	1651	1653	1656	rVB	52136	39664	1.18%	0.152%
28	12.045	1656	1659	1662	rBV	136964	153450	4.55%	0.587%
29	12.227	1687	1690	1693	rBV	61434	49994	1.48%	0.191%
30	12.480	1730	1733	1736	rBV	36706	38587	1.14%	0.148%
31	12.569	1745	1748	1752	rBV	36811	35744	1.06%	0.137%
32	12.645	1758	1761	1765	rBV	736928	648870	19.25%	2.481%
33	12.804	1780	1788	1790	rBV5	23876	41530	1.23%	0.159%
34	12.880	1794	1801	1804	rBV2	496468	573375	17.01%	2.193%
35	12.927	1806	1809	1813	rVB2	31183	37024	1.10%	0.142%
36	13.021	1816	1825	1828	rBV	3141608	2706863	80.30%	10.351%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11944

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.098	1833	1838	1841	rBV3	36331	62964	1.87%	0.241%
38	13.180	1848	1852	1853	rBV2	33025	36785	1.09%	0.141%
39	13.204	1853	1856	1859	rVB	99831	95884	2.84%	0.367%
40	13.269	1864	1867	1870	rBV	79221	70282	2.08%	0.269%
41	13.310	1870	1874	1877	rBV2	51958	54920	1.63%	0.210%
42	13.921	1974	1978	1988	rVB5	96316	188777	5.60%	0.722%
43	14.045	1996	1999	2001	rBV	221845	200511	5.95%	0.767%
44	14.074	2001	2004	2007	rVV2	612813	713417	21.16%	2.728%
45	14.104	2007	2009	2014	rVB	198075	168910	5.01%	0.646%
46	14.463	2066	2070	2073	rBV	37940	35727	1.06%	0.137%
47	15.133	2179	2184	2187	rBV	167858	265574	7.88%	1.016%
48	15.245	2199	2203	2206	rBV	46250	56865	1.69%	0.217%
49	15.445	2233	2237	2244	rBV	91906	137520	4.08%	0.526%
50	15.510	2244	2248	2254	rVB	149801	172768	5.13%	0.661%
51	15.574	2254	2259	2263	rBV	431490	557751	16.55%	2.133%
52	15.851	2301	2306	2312	rBV	215683	364741	10.82%	1.395%
53	17.086	2512	2516	2525	rVB2	65749	135997	4.03%	0.520%
54	17.551	2589	2595	2601	rBV2	47613	94449	2.80%	0.361%

Sum of corrected areas: 26151415

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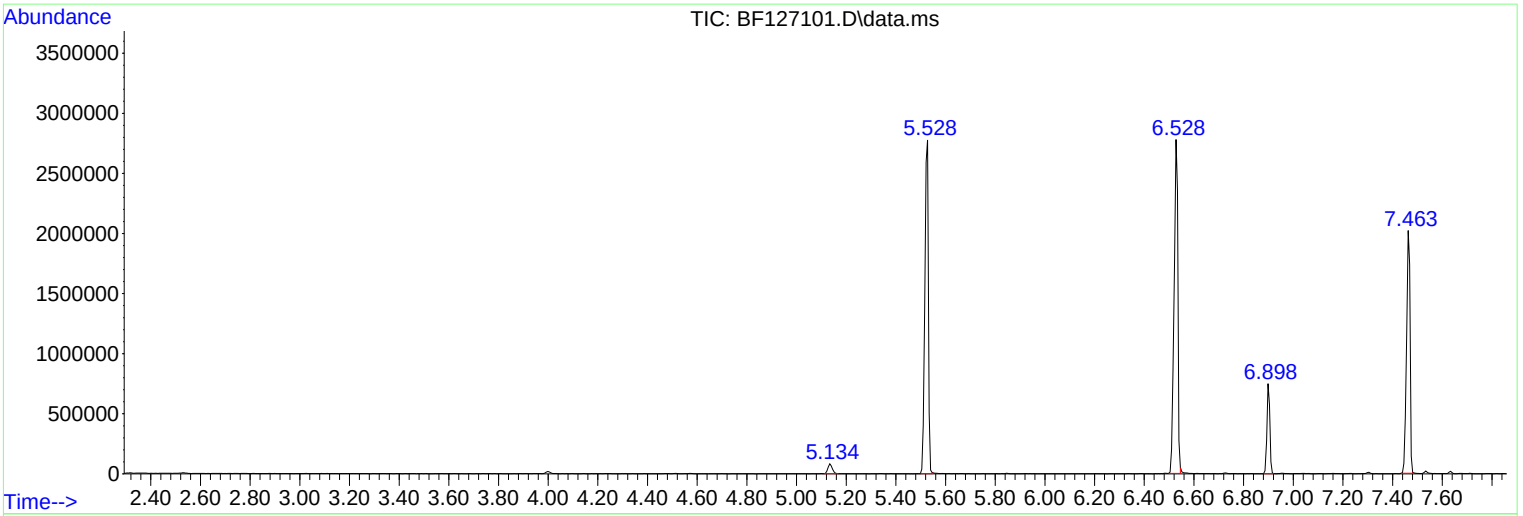
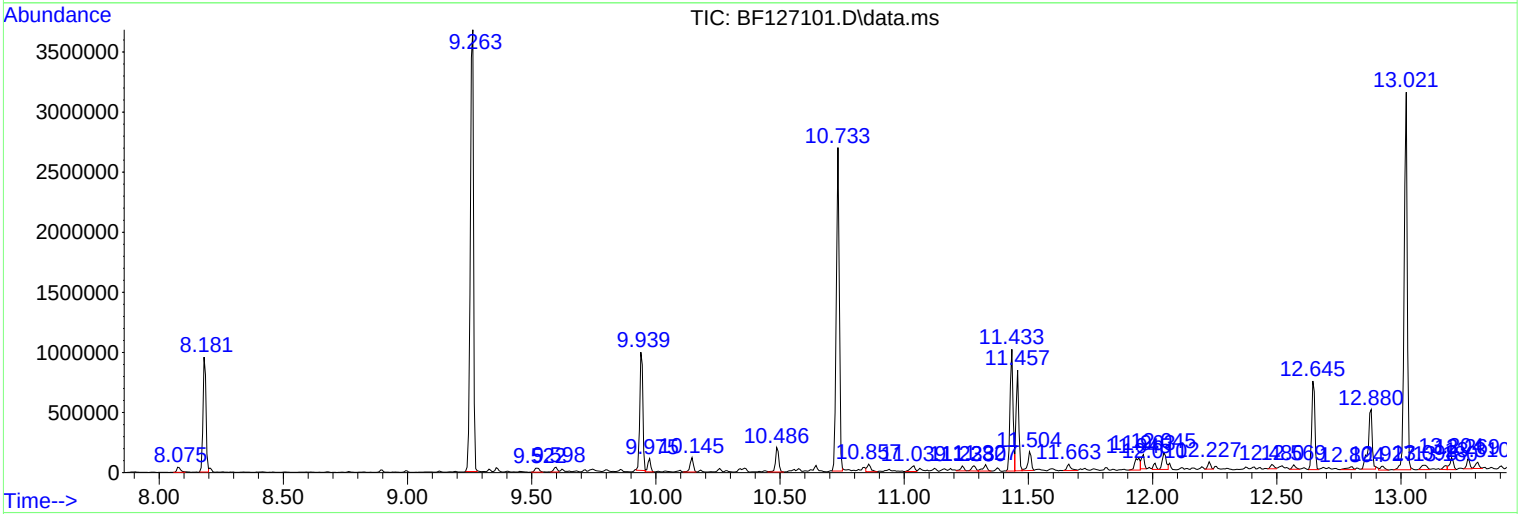
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

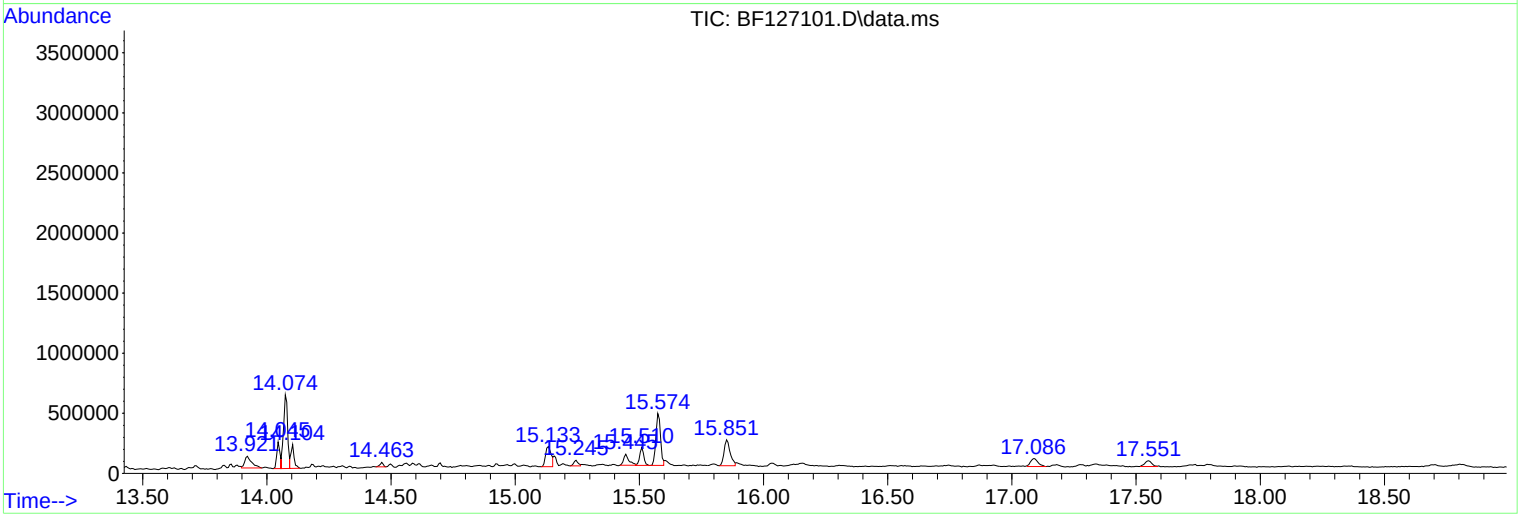
Instrument :
BNA_F
ClientSampleId :
RO-72-11944

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11944

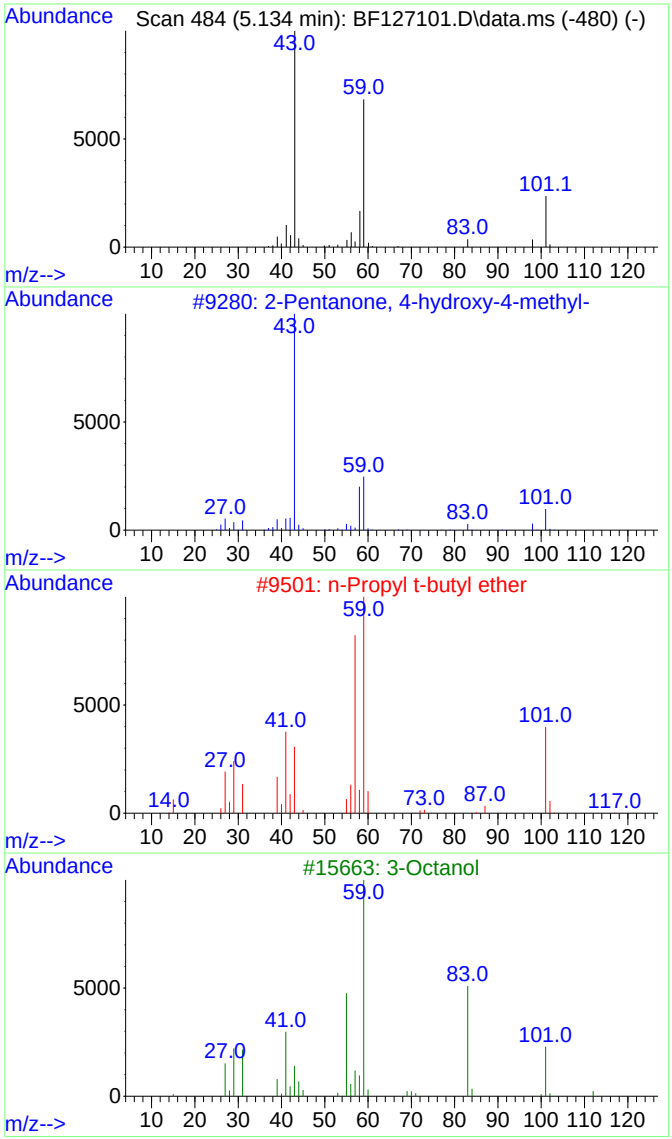
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

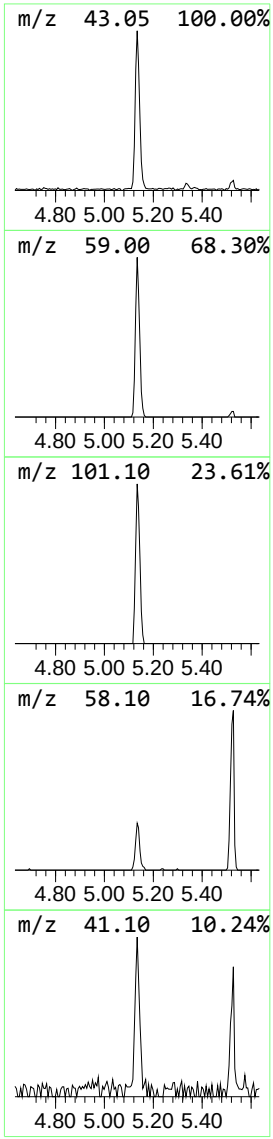
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	3.30 ng	100462	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28
3	3-Octanol	130	C8H18O	000589-98-0	28
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11944

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

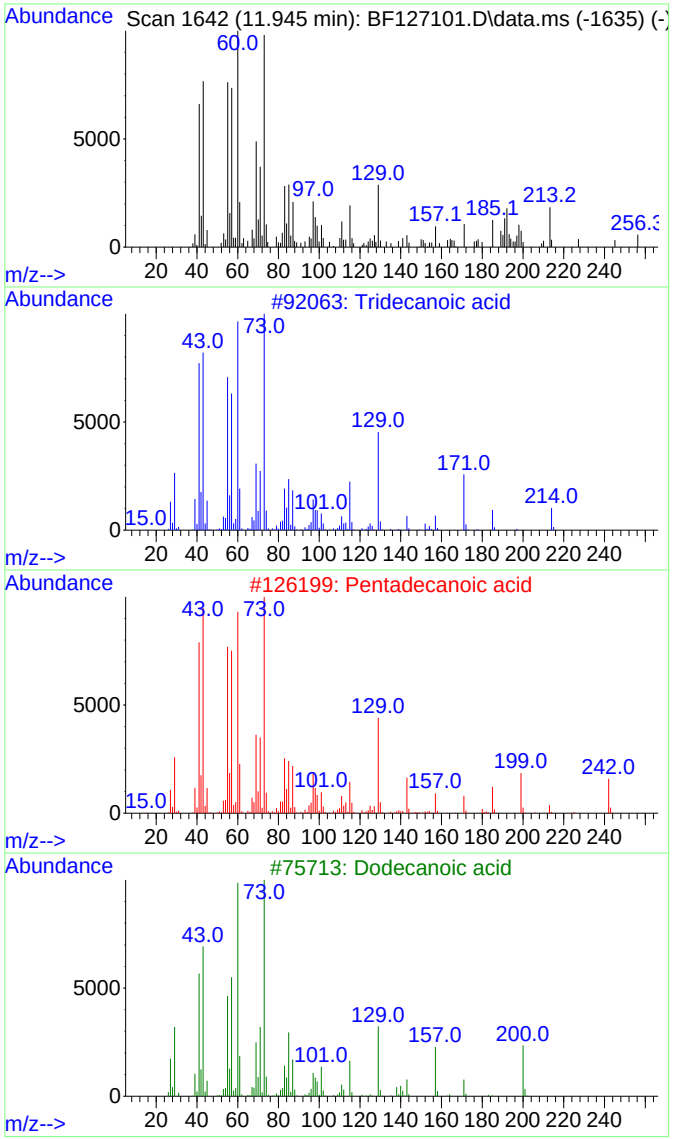
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

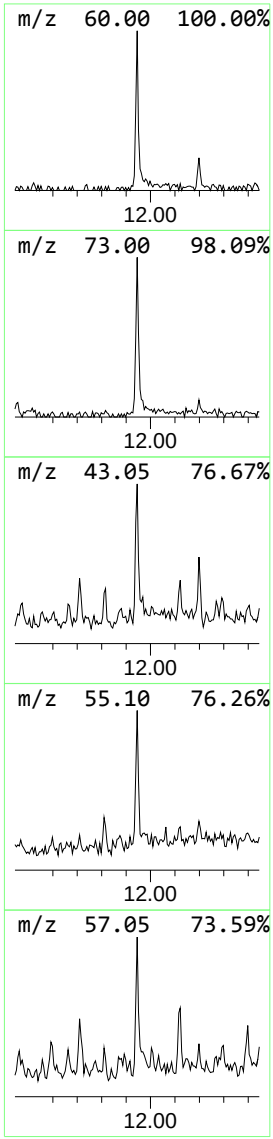
****

Peak Number 2 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	3.47 ng	152753	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Dodecanoic acid	200	C12H24O2	000143-07-7	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11944

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

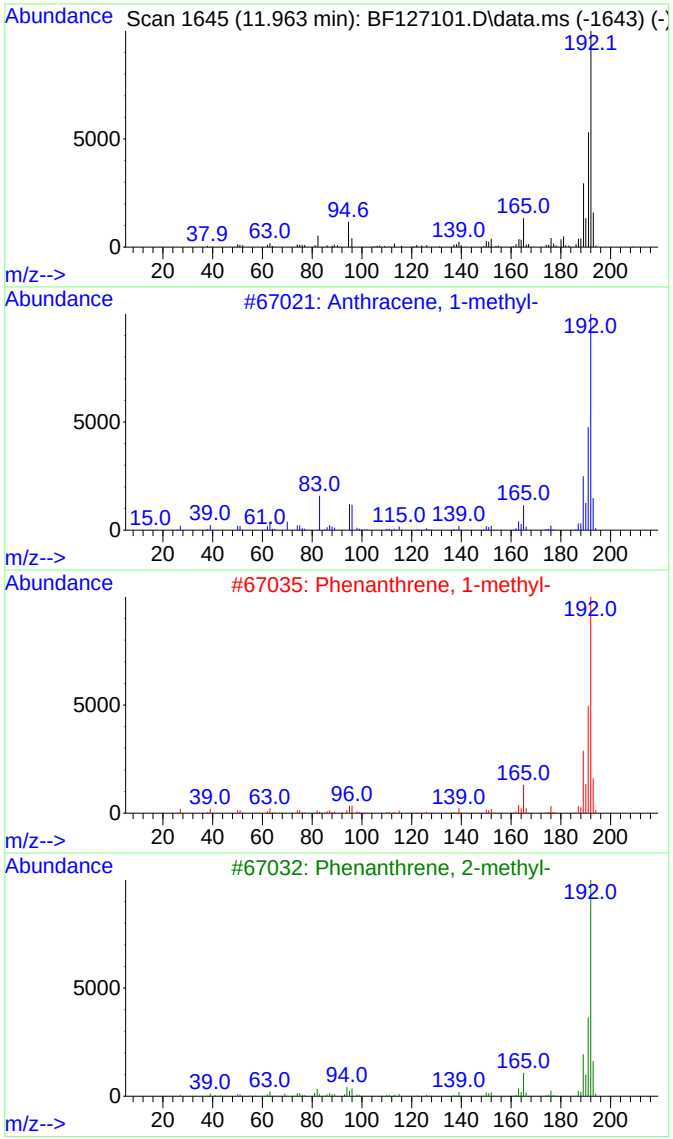
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

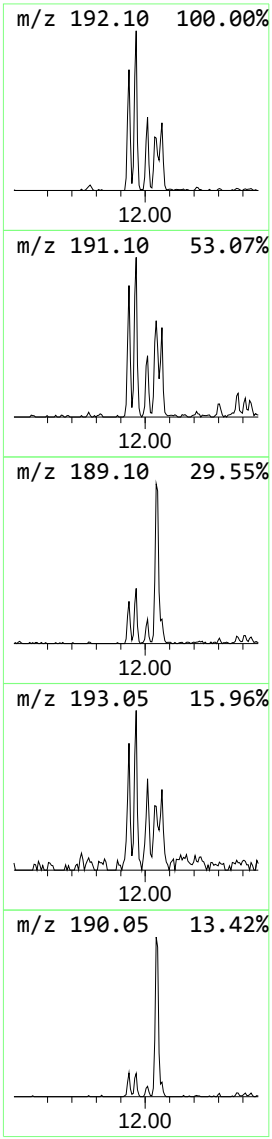
****

Peak Number 3 Anthracene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	2.00 ng	88205	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11944

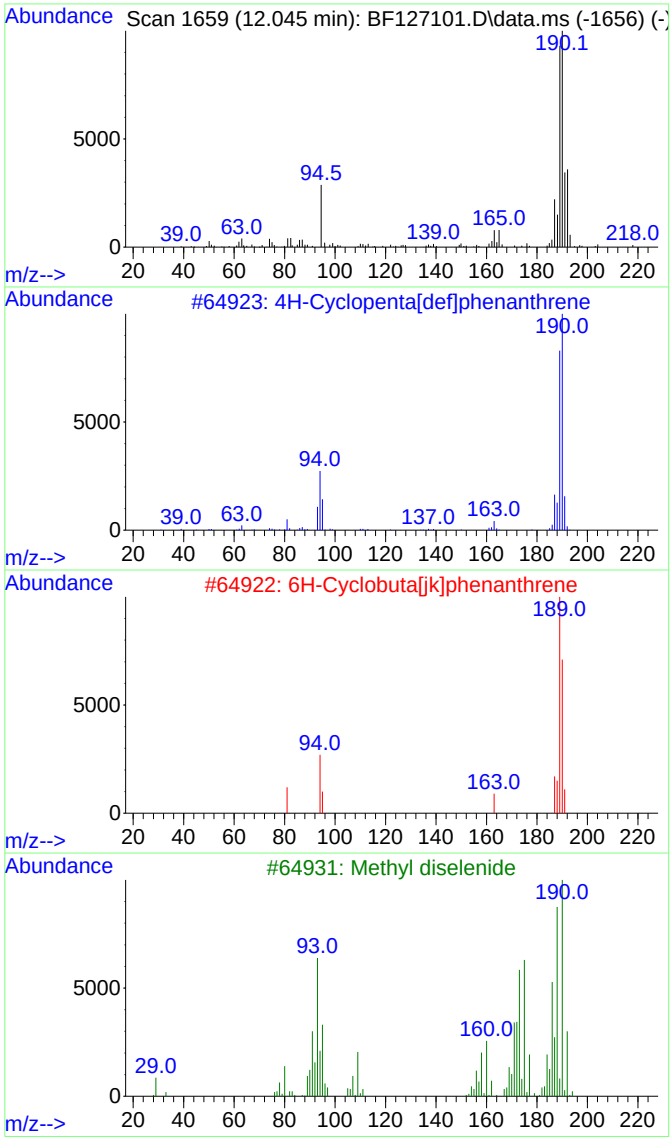
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

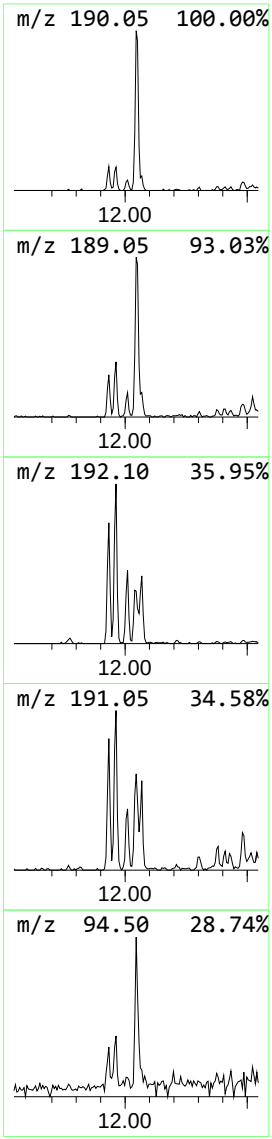
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.045	3.49 ng	153450	Phenanthrene-d10	11.433

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	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	45
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
5	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11944

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

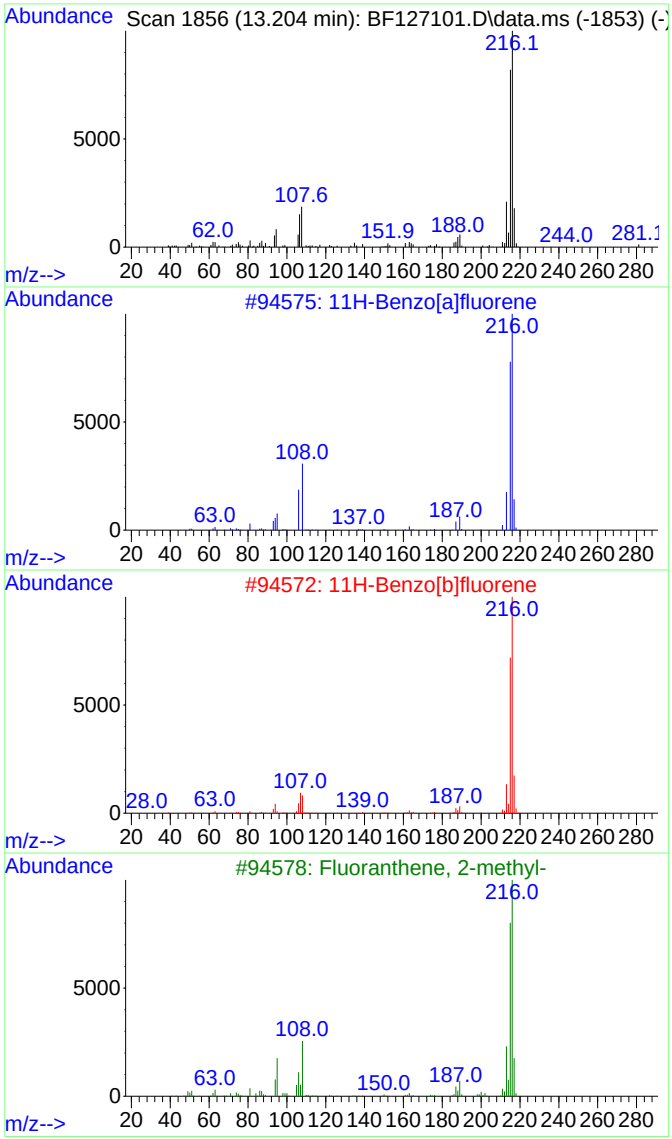
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

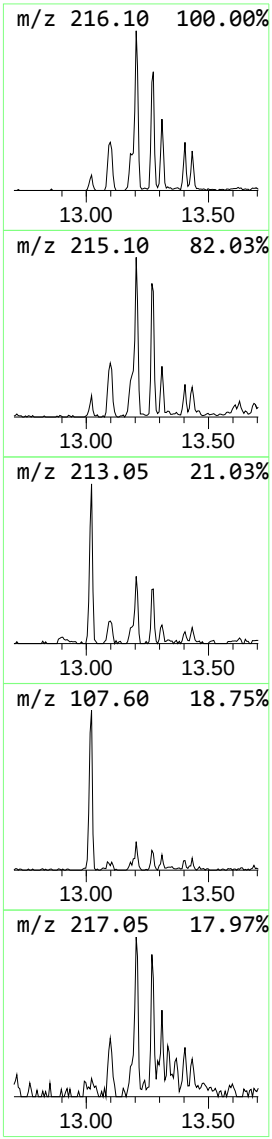
****

Peak Number 5 11H-Benzo[a]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.204	2.69 ng	95884	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	83
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	80
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11944

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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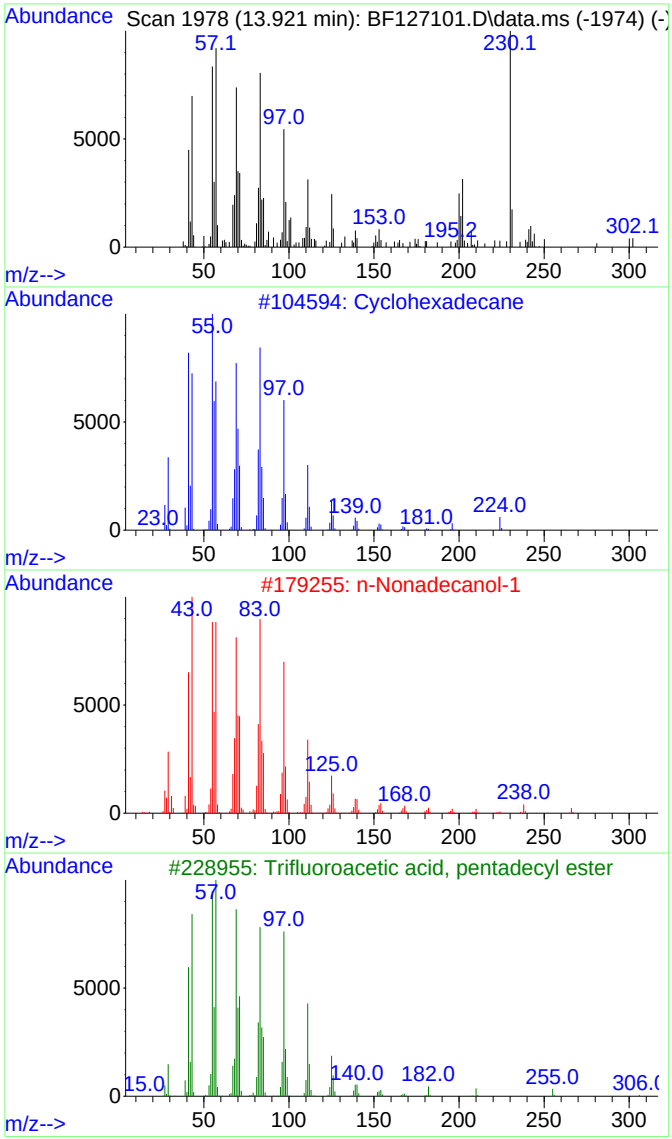
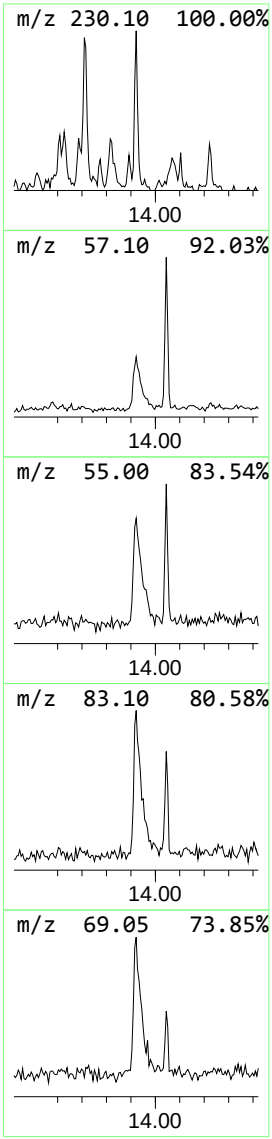
Peak Number 6 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	5.29 ng	188777	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	78
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	64
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	64
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	49
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11944

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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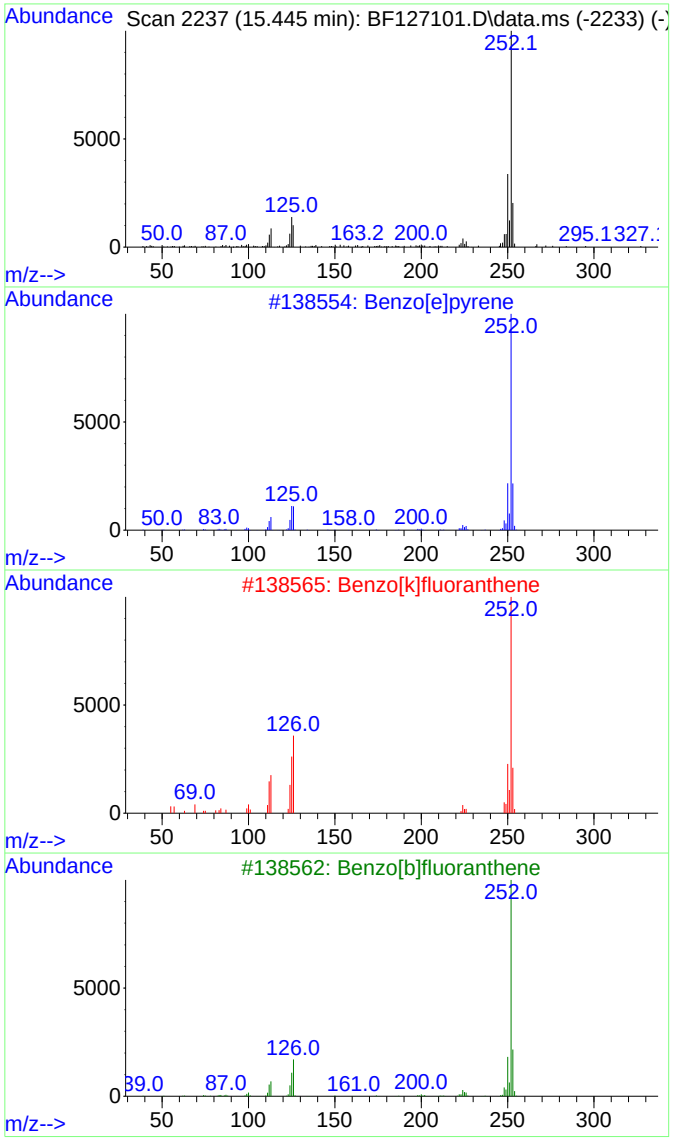
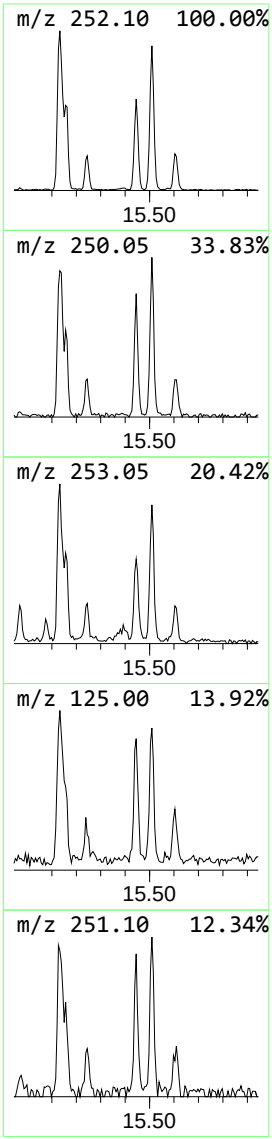
Peak Number 8 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	4.93 ng	137520	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
4	Perylene	252	C20H12	000198-55-0	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11944

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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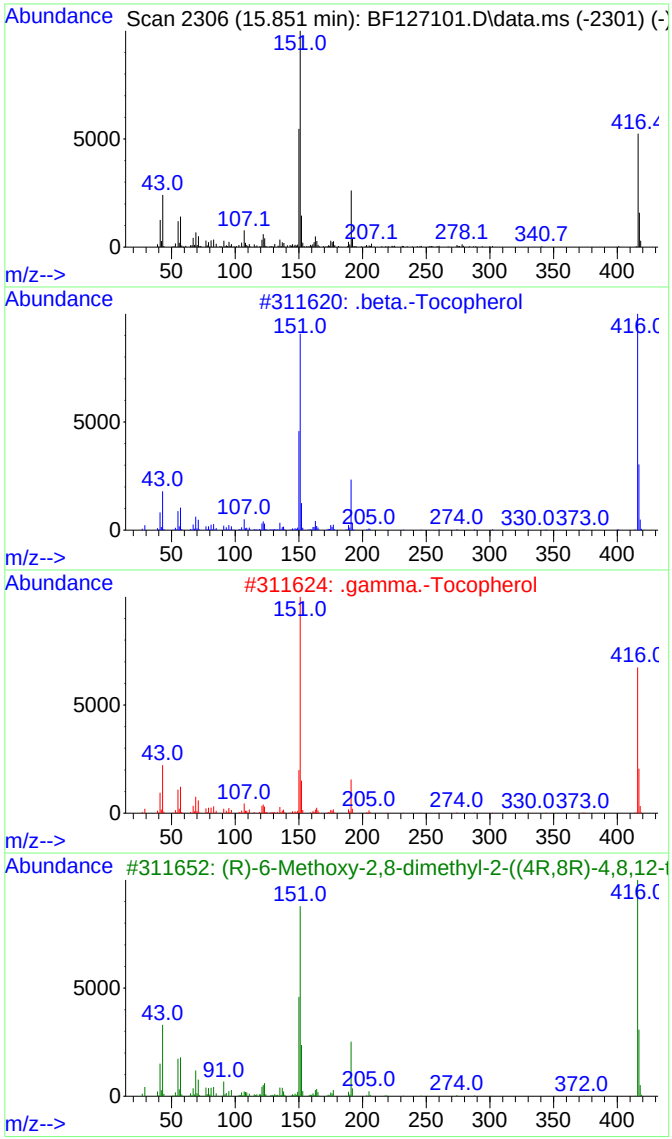
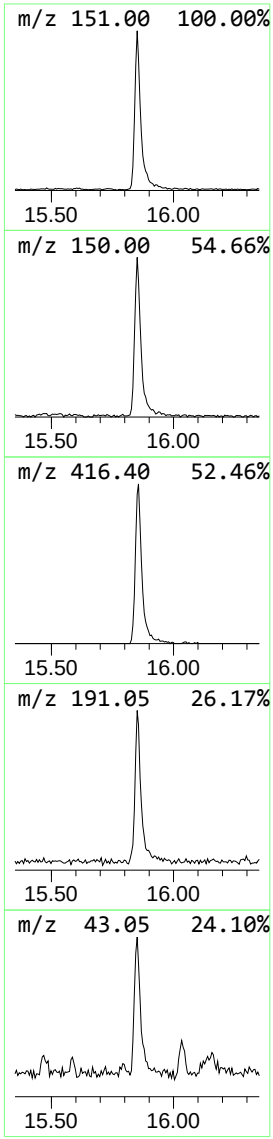
Peak Number 9 .beta.-Tocopherol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.851	13.08 ng	364741	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Tocopherol	416	C28H48O2	000148-03-8	99
2	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	94
3	(R)-6-Methoxy-2,8-dimethyl-2-((4...	416	C28H48O2	1116113-36-0	90
4	Wikstromol, trimethyl ether	416	C23H28O7	1000504-13-5	64
5	3,4-Dihydro-3,5,8-trimethyl-3-(4...	458	C30H50O3	1000105-71-9	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022822\
Data File : BF127101.D
Acq On : 28 Feb 2022 15:50
Operator : CG\JU
Sample : N1679-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11944

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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-...	5.134	3.3	ng	100462	1	6.898	608343	20.0
Tridecanoic acid	11.945	3.5	ng	152753	4	11.433	880236	20.0
Anthracene, 1-m...	11.963	2.0	ng	88205	4	11.433	880236	20.0
4H-Cyclopenta[d...	12.045	3.5	ng	153450	4	11.433	880236	20.0
11H-Benzo[a]flu...	13.204	2.7	ng	95884	5	14.080	713417	20.0
Cyclohexadecane	13.921	5.3	ng	188777	5	14.080	713417	20.0
Benzo[e]pyrene	15.445	4.9	ng	137520	6	15.574	557751	20.0
.beta.-Tocopherol	15.851	13.1	ng	364741	6	15.574	557751	20.0