LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051822\
Data File : BF128325.D
Acq On : 18 May 2022 21:53
Operator : CG\JU
Sample : N2900-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-051722

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-BF050922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128325.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	472	475	482	rVB	50570	54756	4.77%	0.466%
2	5.487	541	544	558	rBV	916792	849437	73.96%	7.226%
3	6.498	712	716	733	rBV	1141522	961855	83.75%	8.183%
4	6.869	775	779	786	rBV	564809	461163	40.15%	3.923%
5	7.434	871	875	878	rBV	827756	681703	59.36%	5.799%
6	8.151	993	997	1001	rBV	687337	561263	48.87%	4.775%
7	9.228	1175	1180	1183	rBV	1254674	1148517	100.00%	9.771%
8	9.292	1187	1191	1195	rVV	20017	20174	1.76%	0.172%
9	9.910	1292	1296	1299	rBV	654848	546046	47.54%	4.645%
10	10.698	1427	1430	1440	rBV	514483	445773	38.81%	3.792%
11	10.798	1443	1447	1452	rVV3	8189	12903	1.12%	0.110%
12	11.398	1546	1549	1552	rBV	585128	494857	43.09%	4.210%
13	11.422	1552	1553	1557	rVB	83042	53307	4.64%	0.453%
14	11.474	1557	1562	1567	rBV	21763	20332	1.77%	0.173%
15	11.780	1610	1614	1617	rBV	128879	110710	9.64%	0.942%
16	11.898	1631	1634	1637	rBV	13220	13865	1.21%	0.118%
17	11.927	1637	1639	1643	rVB	19973	18275	1.59%	0.155%
18	12.016	1651	1654	1656	rBV	30709	29881	2.60%	0.254%
19	12.227	1687	1690	1696	rVB6	13016	13431	1.17%	0.114%
20	12.469	1725	1731	1732	rBV	780271	677320	58.97%	5.762%
21	12.486	1732	1734	1740	rVV2	557128	501421	43.66%	4.266%
22	12.545	1740	1744	1746	rVV3	18746	21460	1.87%	0.183%
23	12.569	1746	1748	1752	rVB	118057	101090	8.80%	0.860%
24	12.616	1752	1756	1760	rBV	326918	272241	23.70%	2.316%
25	12.845	1789	1795	1801	rBV	281885	297400	25.89%	2.530%
26	12.892	1801	1803	1807	rVB4	15351	17888	1.56%	0.152%
27	12.986	1811	1819	1822	rBV	1090869	1034692	90.09%	8.802%
28	13.063	1828	1832	1836	rBV2	20790	35016	3.05%	0.298%
29	13.174	1844	1851	1853	rBV	43901	64539	5.62%	0.549%
30	13.198	1853	1855	1857	rBV3	14991	13743	1.20%	0.117%
31	13.239	1860	1862	1865	rVB2	31494	26105	2.27%	0.222%
32	13.280	1865	1869	1870	rBV3	32234	37841	3.29%	0.322%
33	13.374	1882	1885	1887	rBV	16334	14126	1.23%	0.120%
34	13.404	1887	1890	1897	rVB6	19013	30457	2.65%	0.259%
35	13.545	1912	1914	1917	rBV2	17490	17518	1.53%	0.149%
36	13.686	1936	1938	1940	rBV	23556	20257	1.76%	0.172%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051822\
Data File : BF128325.D
Acq On : 18 May 2022 21:53
Operator : CG\JU
Sample : N2900-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-051722

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-BF050922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.798	1954	1957	1959	rBV2	27549	24605	2.14%	0.209%
38	13.821	1959	1961	1963	rVB	25739	17619	1.53%	0.150%
39	13.851	1963	1966	1967	rBV	22546	23715	2.06%	0.202%
40	13.898	1968	1974	1981	rVB6	86651	184238	16.04%	1.567%
41	13.968	1983	1986	1990	rBV5	20370	23759	2.07%	0.202%
42	14.045	1994	1999	2002	rBV2	626339	723443	62.99%	6.154%
43	14.074	2002	2004	2011	rVB	142601	134954	11.75%	1.148%
44	14.133	2012	2014	2016	rBV2	24859	28171	2.45%	0.240%
45	15.098	2175	2178	2181	rBV	131165	177850	15.49%	1.513%
46	15.410	2228	2231	2237	rVB	74840	87618	7.63%	0.745%
47	15.474	2238	2242	2247	rVB	121685	157091	13.68%	1.336%
48	15.539	2248	2253	2257	rBV2	389079	490388	42.70%	4.172%

Sum of corrected areas: 11754813

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051822\
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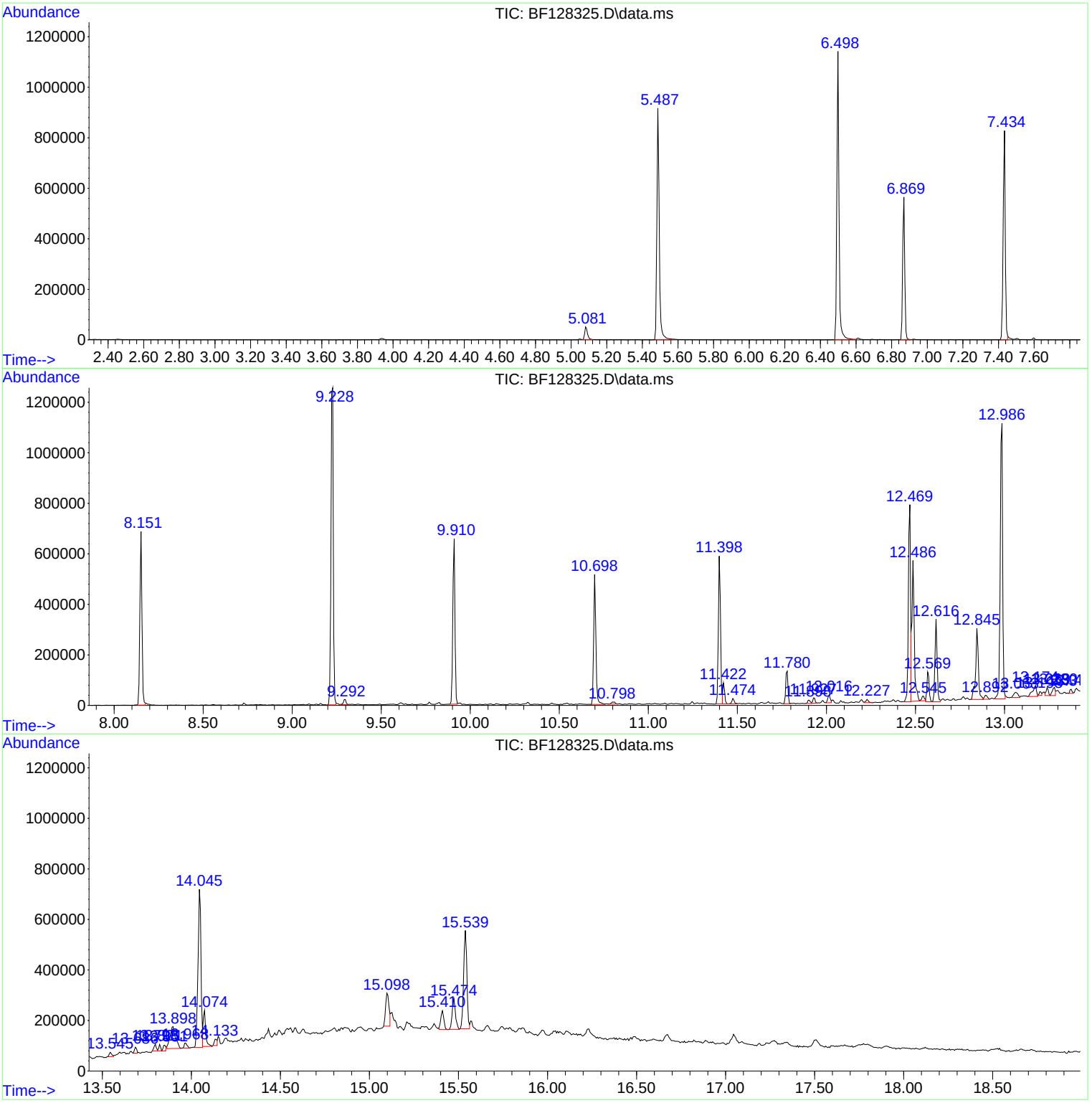
Operator : CG\JU
Sample : N2900-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-051722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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\BF051822\
Data File : BF128325.D
Acq On : 18 May 2022 21:53
Operator : CG\JU
Sample : N2900-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-051722

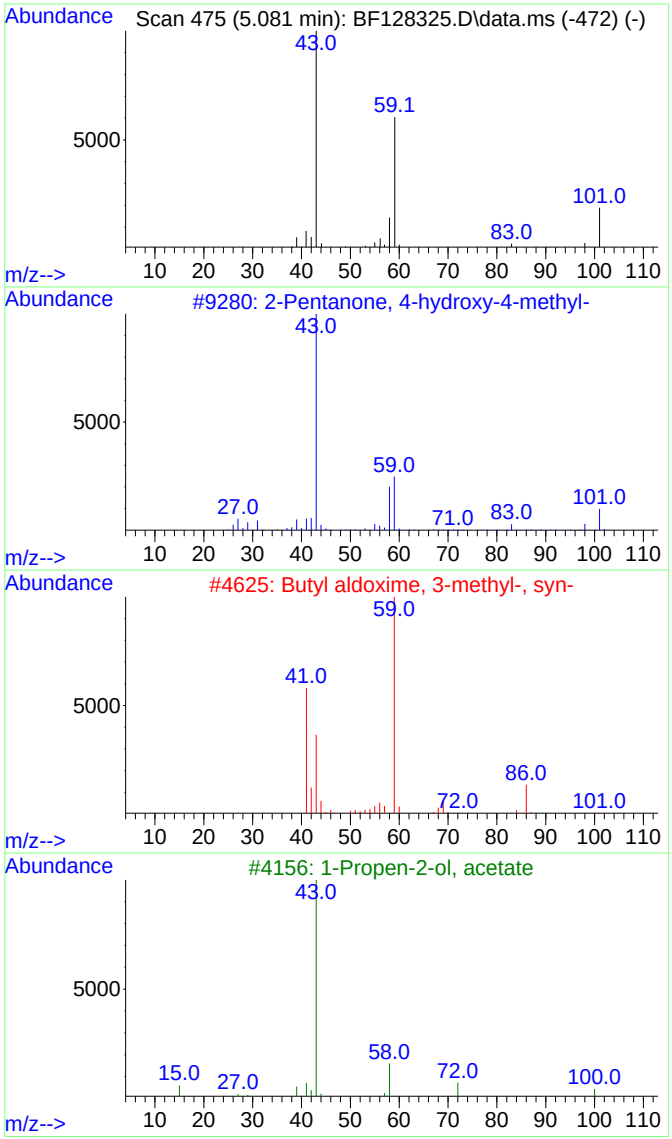
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

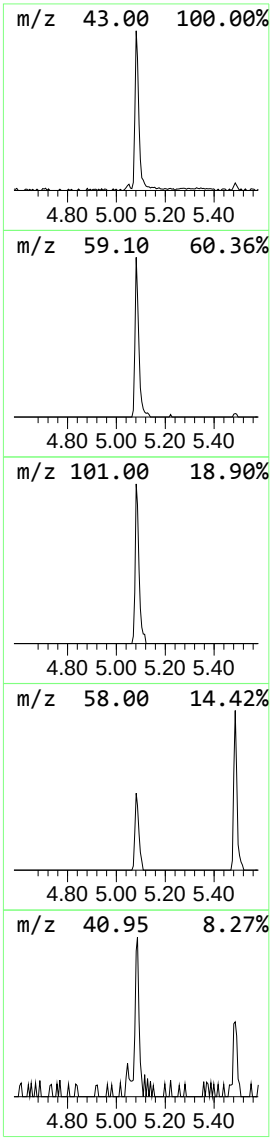
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	2.37 ng	54756	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051822\
Data File : BF128325.D
Acq On : 18 May 2022 21:53
Operator : CG\JU
Sample : N2900-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-051722

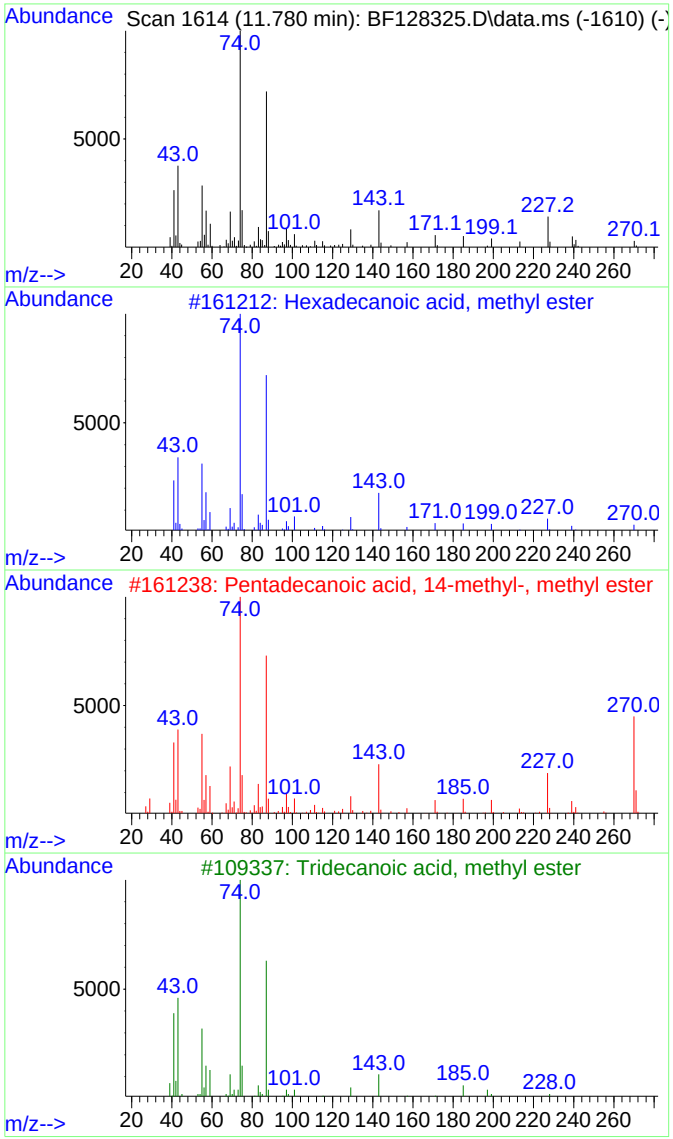
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

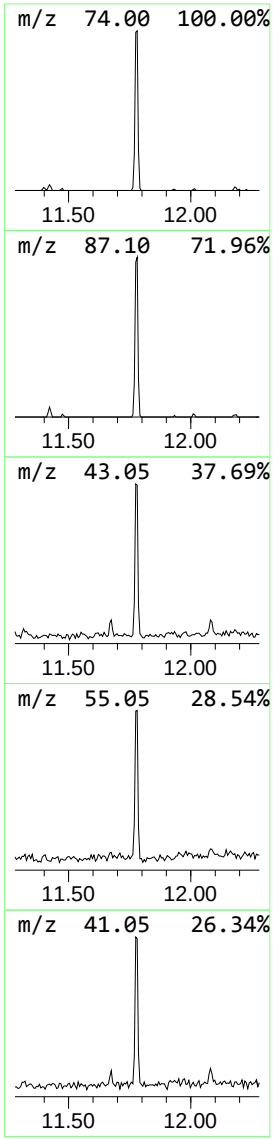
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	4.47 ng	110710	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051822\
Data File : BF128325.D
Acq On : 18 May 2022 21:53
Operator : CG\JU
Sample : N2900-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-051722

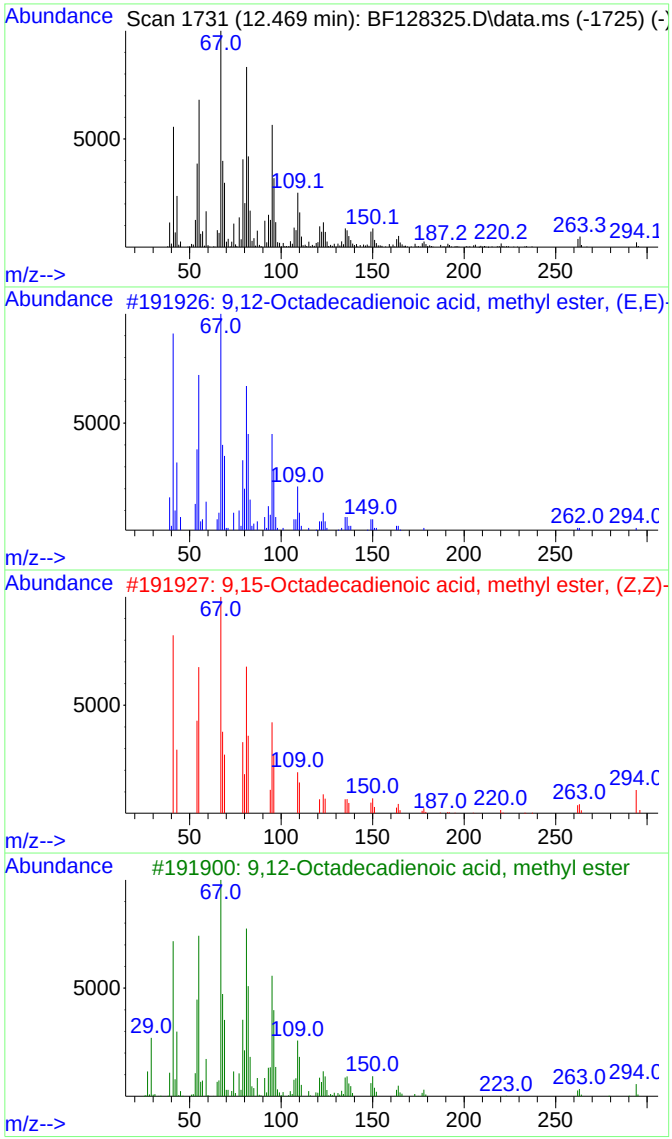
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

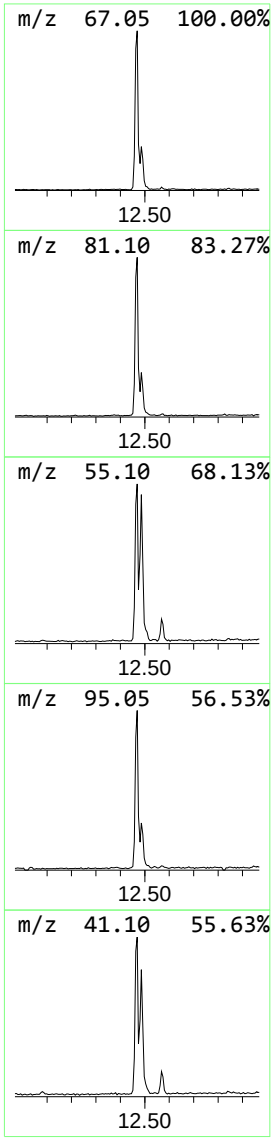
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	27.37 ng	677320	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051822\
Data File : BF128325.D
Acq On : 18 May 2022 21:53
Operator : CG\JU
Sample : N2900-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-051722

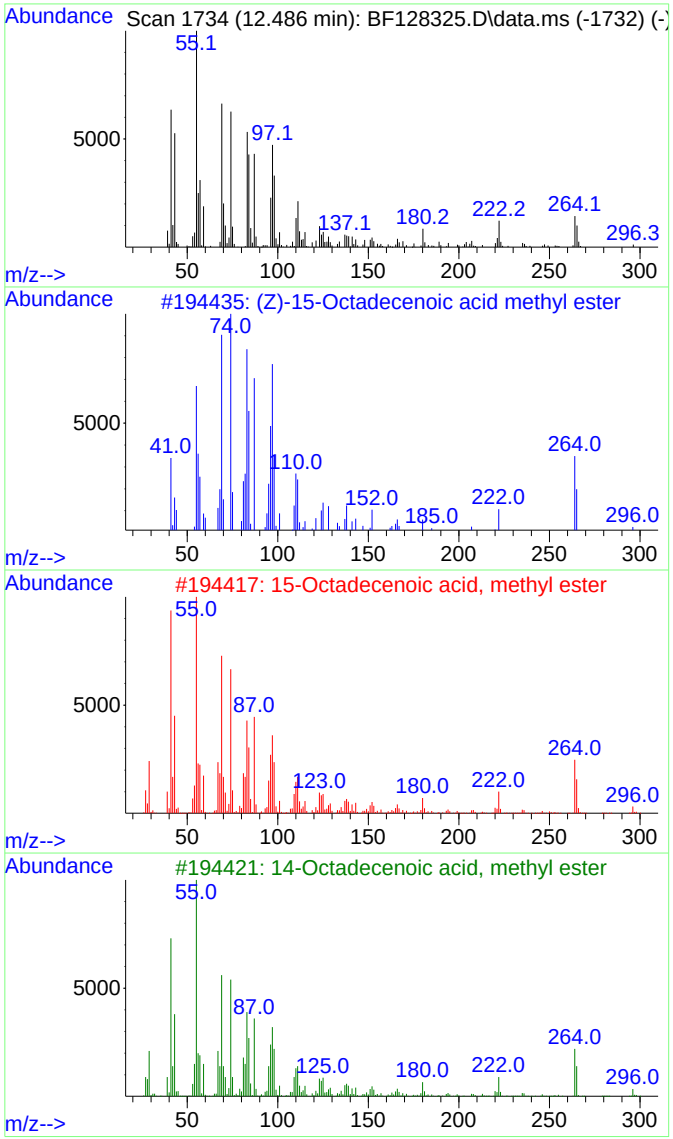
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

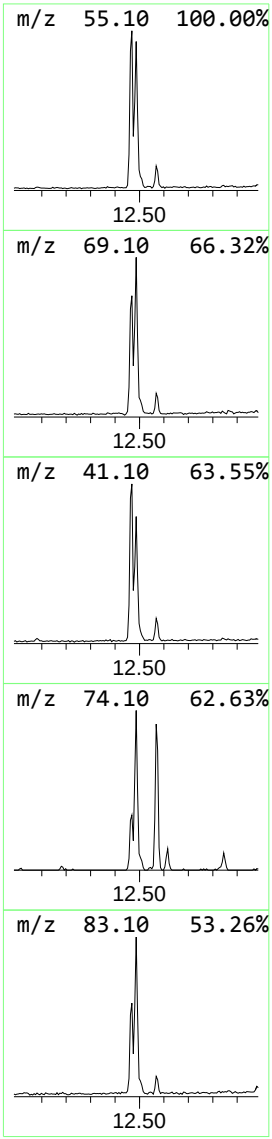
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (Z)-15-Octadecenoic acid me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.486	20.27 ng	501421	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	98
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	96
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	93
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	93
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051822\
Data File : BF128325.D
Acq On : 18 May 2022 21:53
Operator : CG\JU
Sample : N2900-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

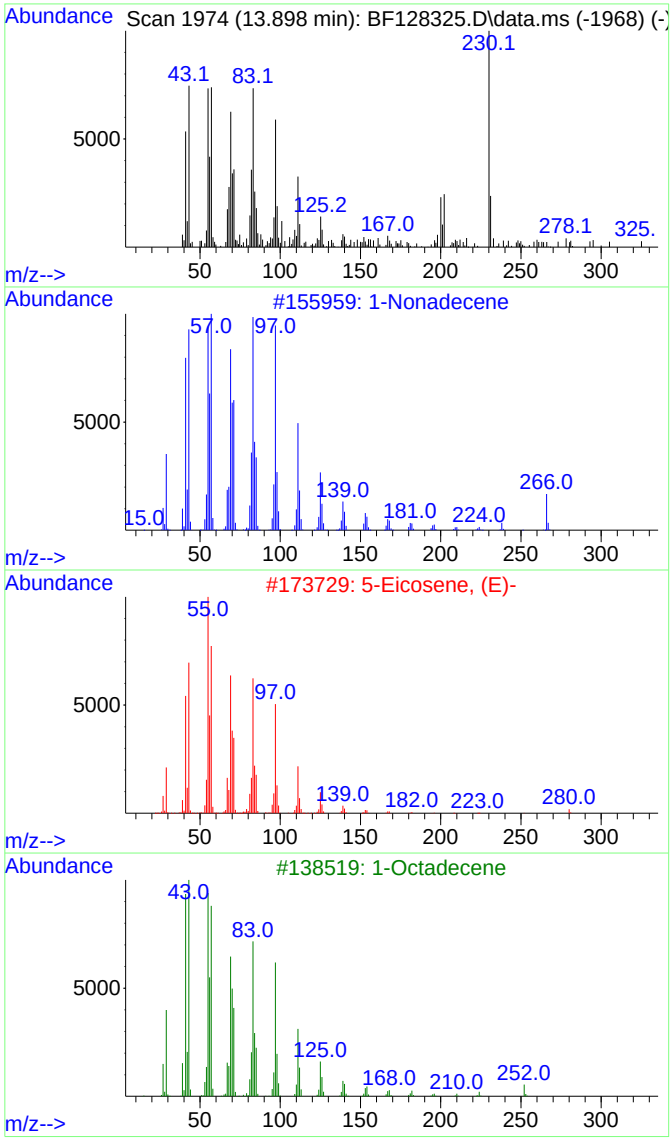
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

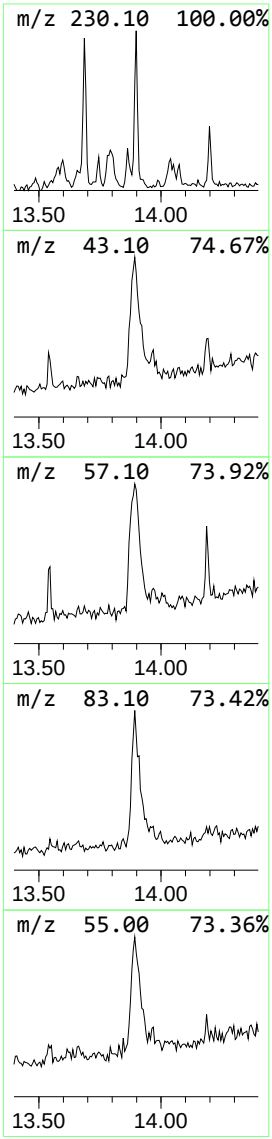
****

Peak Number 5 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.09 ng	184238	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	97
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
3	1-Octadecene	252	C18H36	000112-88-9	96
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
5	Cyclopentadecane	210	C15H30	000295-48-7	95





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Data File : BF128325.D
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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

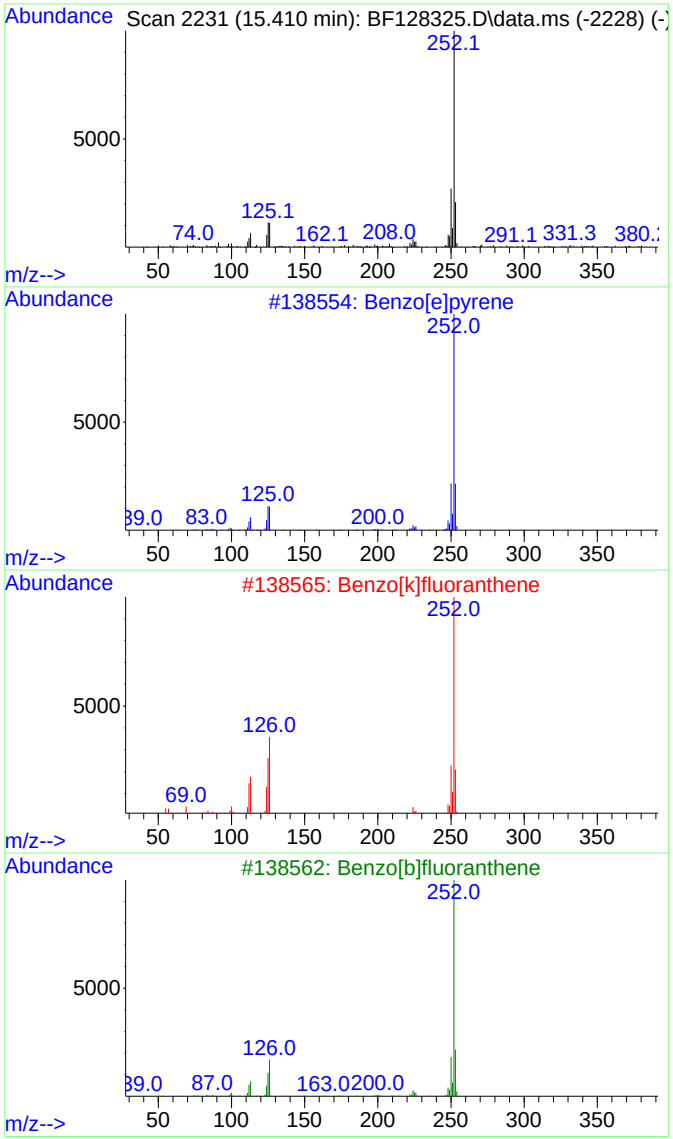
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

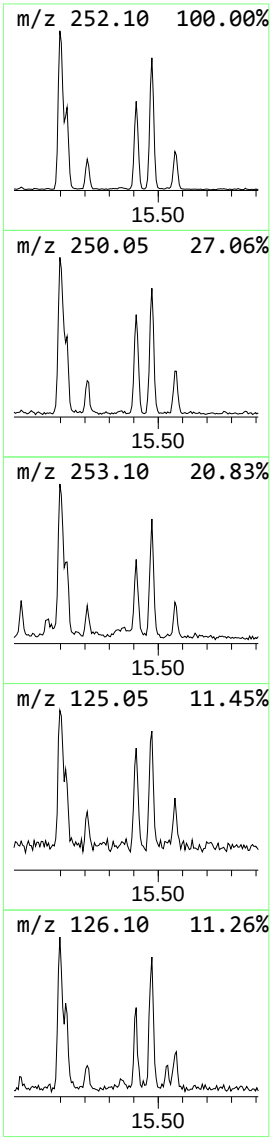
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	3.57 ng	87618	Perylene-d12	15.539

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	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051822\
Data File : BF128325.D
Acq On : 18 May 2022 21:53
Operator : CG\JU
Sample : N2900-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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-...	5.081	2.4	ng	54756	1	6.869	461163	20.0
Hexadecanoic ac...	11.780	4.5	ng	110710	4	11.398	494857	20.0
9,12-Octadecadi...	12.469	27.4	ng	677320	4	11.398	494857	20.0
(Z)-15-Octadece...	12.486	20.3	ng	501421	4	11.398	494857	20.0
1-Nonadecene	13.898	5.1	ng	184238	5	14.045	723443	20.0
Benzo[e]pyrene	15.410	3.6	ng	87618	6	15.539	490388	20.0