LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125333.D
Acq On : 2 Sep 2021 21:48
Operator : JU/CG
Sample : M3636-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-01-090121

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125333.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	6	11	18	rVB	205498	259500	14.31%	1.287%
2	5.516	579	583	596	rBV	725485	681322	37.58%	3.378%
3	6.528	751	755	763	rBV	760847	694046	38.28%	3.441%
4	6.904	816	819	823	rBV	1177287	963766	53.16%	4.778%
5	7.463	911	914	925	rBV	431695	438932	24.21%	2.176%
6	8.128	1020	1027	1034	rBV5	8938	30687	1.69%	0.152%
7	8.192	1034	1038	1045	rBV	1447148	1267646	69.92%	6.285%
8	9.263	1216	1220	1231	rBV	1010185	847572	46.75%	4.202%
9	9.945	1333	1336	1348	rVB	1656594	1470225	81.10%	7.289%
10	10.369	1400	1408	1410	rBV	24385	23529	1.30%	0.117%
11	10.733	1467	1470	1481	rVB	547313	492593	27.17%	2.442%
12	10.839	1486	1488	1494	rBV2	35540	45301	2.50%	0.225%
13	11.292	1560	1565	1567	rBV2	46515	47176	2.60%	0.234%
14	11.316	1567	1569	1576	rVB3	23665	34881	1.92%	0.173%
15	11.433	1586	1589	1592	rBV	1489316	1384205	76.35%	6.863%
16	11.457	1592	1593	1597	rVV	227533	161349	8.90%	0.800%
17	11.510	1599	1602	1605	rVB	60611	53562	2.95%	0.266%
18	11.716	1634	1637	1639	rBV	45163	38040	2.10%	0.189%
19	11.745	1639	1642	1644	rVB2	37432	31664	1.75%	0.157%
20	11.822	1651	1655	1658	rBV	1354935	1154452	63.68%	5.724%
21	11.951	1671	1677	1685	rBV2	90406	164720	9.09%	0.817%
22	12.051	1690	1694	1696	rBV	49904	51226	2.83%	0.254%
23	12.122	1703	1706	1709	rBV	41583	42880	2.37%	0.213%
24	12.227	1721	1724	1727	rBV2	34476	42040	2.32%	0.208%
25	12.504	1768	1771	1773	rBV	1259891	1167679	64.41%	5.789%
26	12.527	1773	1775	1778	rVV	2182575	1812943	100.00%	8.988%
27	12.574	1781	1783	1786	rVB	45330	37407	2.06%	0.185%
28	12.610	1786	1789	1792	rBV	681432	537610	29.65%	2.665%
29	12.651	1792	1796	1801	rBV	538159	492760	27.18%	2.443%
30	12.739	1809	1811	1815	rBV5	20378	21354	1.18%	0.106%
31	12.880	1832	1835	1841	rVB	474584	422692	23.32%	2.096%
32	12.927	1841	1843	1848	rVB2	27142	33230	1.83%	0.165%
33	13.016	1852	1858	1862	rBV	766045	676568	37.32%	3.354%
34	13.098	1867	1872	1876	rBV4	40765	75993	4.19%	0.377%
35	13.180	1882	1886	1888	rBV4	47015	68414	3.77%	0.339%
36	13.204	1888	1890	1894	rVV	61741	70276	3.88%	0.348%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125333.D
Acq On : 2 Sep 2021 21:48
Operator : JU/CG
Sample : M3636-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-01-090121

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.245	1894	1897	1898	rVV	31845	36682	2.02%	0.182%
38	13.274	1898	1902	1905	rVV3	54789	96353	5.31%	0.478%
39	13.310	1905	1908	1910	rVV2	57115	72496	4.00%	0.359%
40	13.339	1910	1913	1916	rVB	62227	58664	3.24%	0.291%
41	13.404	1922	1924	1927	rBV	24059	23432	1.29%	0.116%
42	13.445	1927	1931	1936	rVB2	163889	179317	9.89%	0.889%
43	13.586	1952	1955	1958	rBV4	24985	29686	1.64%	0.147%
44	13.716	1974	1977	1981	rBV	72274	69310	3.82%	0.344%
45	13.769	1982	1986	1990	rVB7	42215	59723	3.29%	0.296%
46	13.827	1992	1996	1999	rBV2	54937	75770	4.18%	0.376%
47	13.857	1999	2001	2003	rVV	35151	33337	1.84%	0.165%
48	13.880	2003	2005	2009	rVV2	33885	44475	2.45%	0.221%
49	13.921	2009	2012	2016	rVB	50985	53863	2.97%	0.267%
50	14.080	2034	2039	2041	rBV2	1197644	1289270	71.11%	6.392%
51	14.104	2041	2043	2050	rVB	258555	245555	13.54%	1.217%
52	14.186	2055	2057	2059	rVB	33459	25052	1.38%	0.124%
53	14.463	2102	2104	2107	rVB	57396	49401	2.72%	0.245%
54	15.133	2214	2218	2222	rBV	232660	391521	21.60%	1.941%
55	15.245	2235	2237	2242	rBV	41161	40772	2.25%	0.202%
56	15.451	2269	2272	2277	rVB	137154	161066	8.88%	0.799%
57	15.510	2279	2282	2288	rVV	171104	225591	12.44%	1.118%
58	15.580	2289	2294	2309	rVB	768185	1070244	59.03%	5.306%

Sum of corrected areas: 20169820

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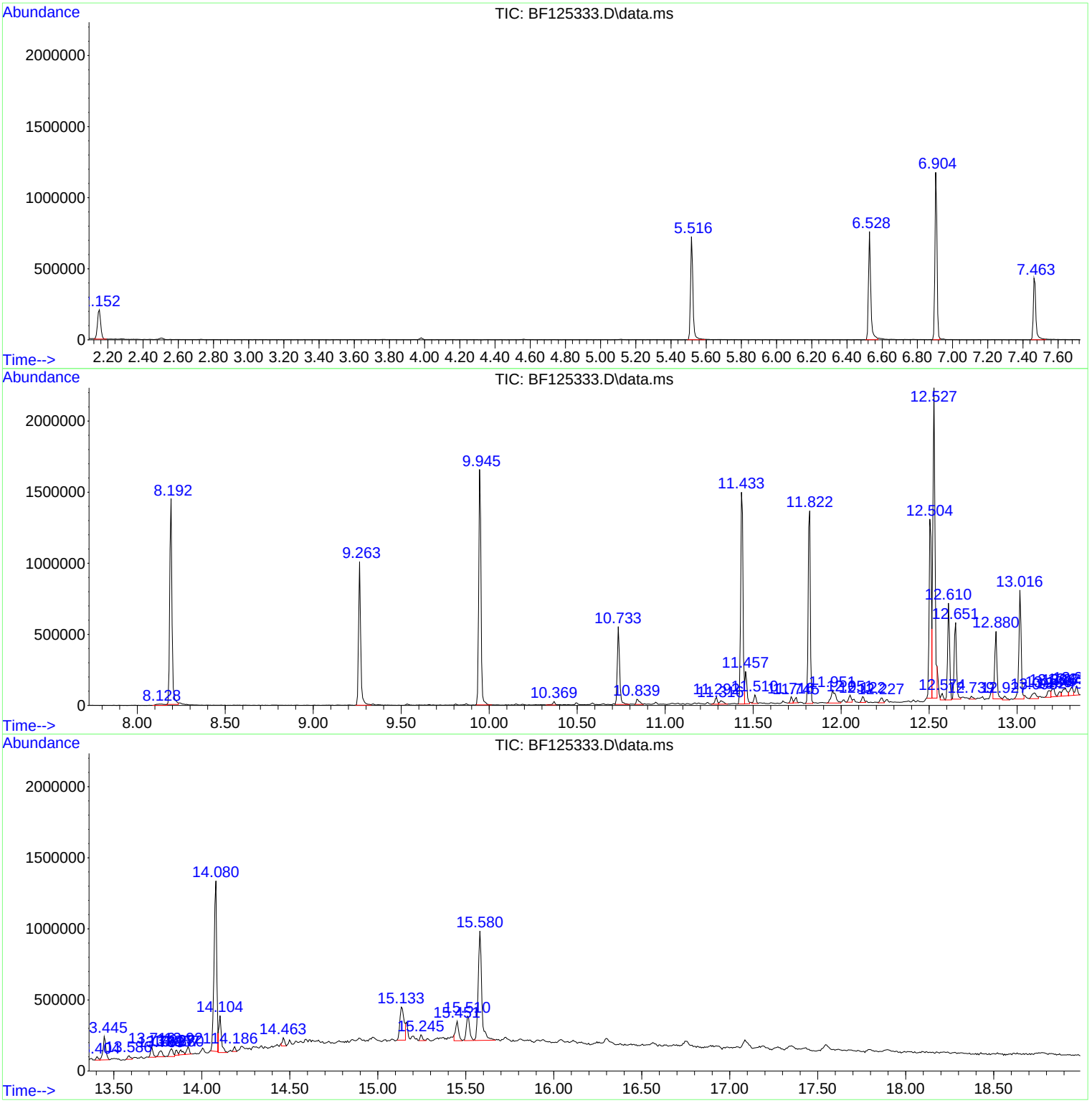
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-090121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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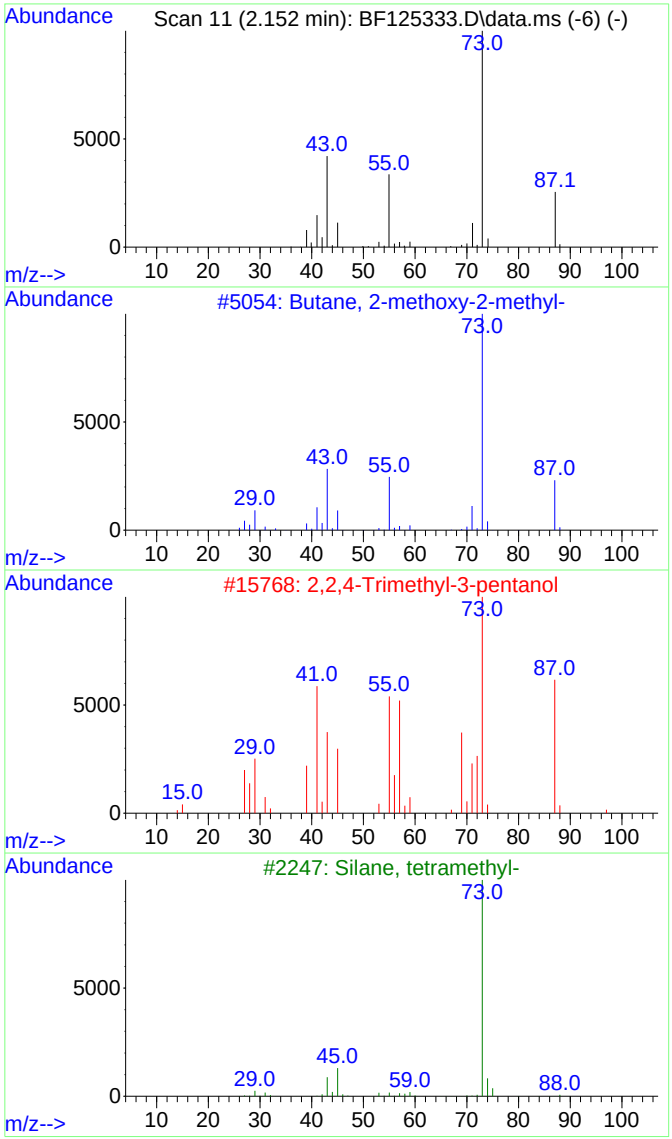
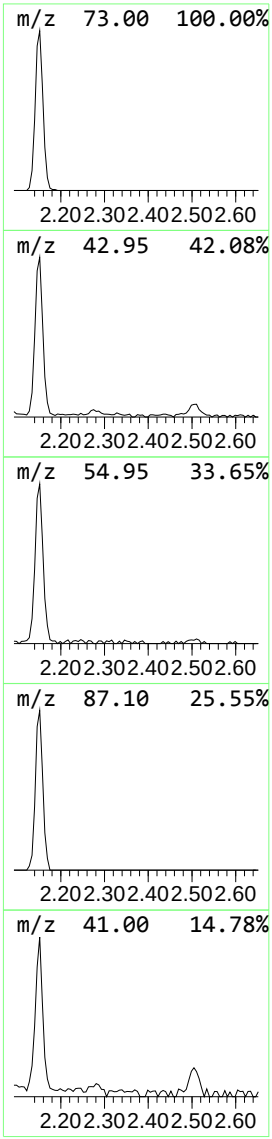
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	5.39 ng	259500	1,4-Dichlorobenzene-d4	6.904

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	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25





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Data File : BF125333.D
Acq On : 2 Sep 2021 21:48
Operator : JU/CG
Sample : M3636-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-090121

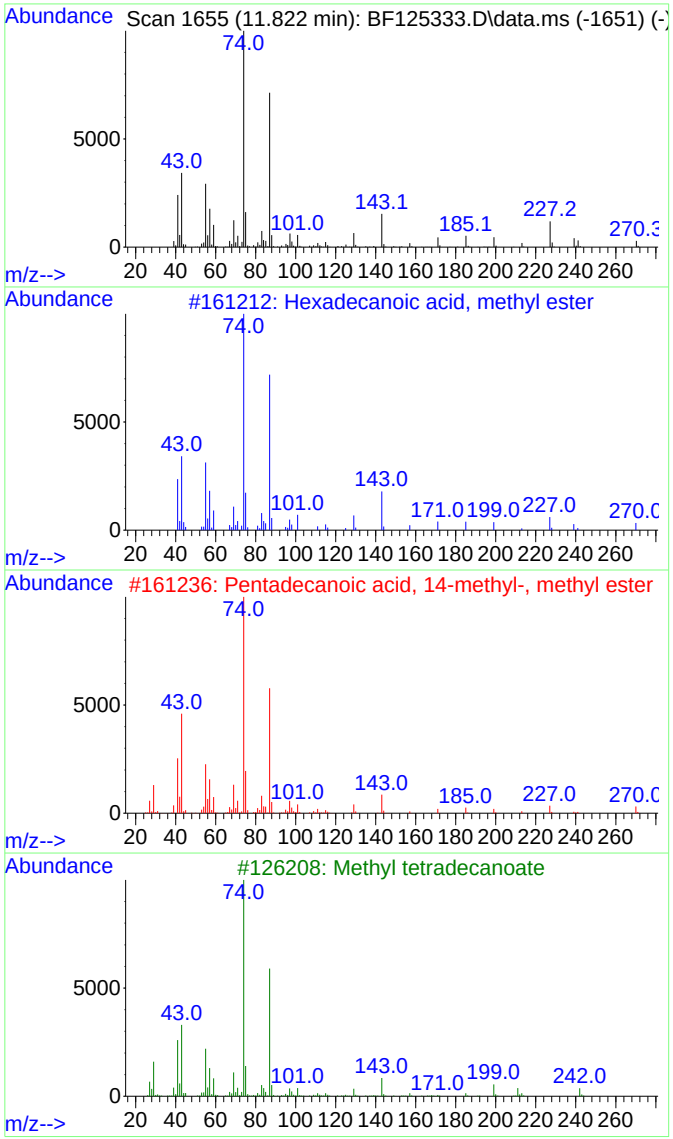
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

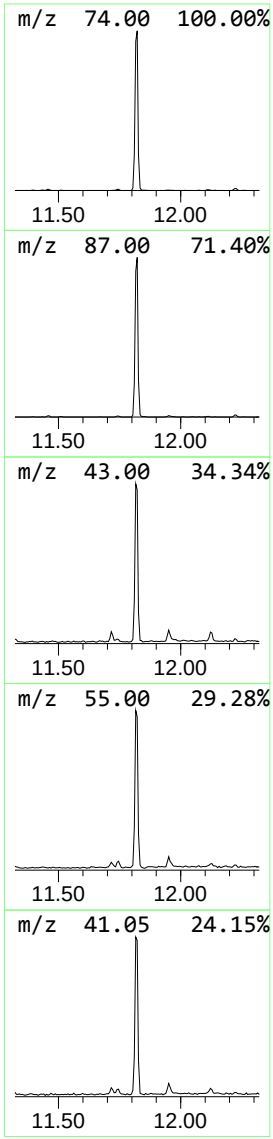
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	16.68 ng	1154450	Phenanthrene-d10	11.433

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	96
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	94
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	89
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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Operator : JU/CG
Sample : M3636-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-090121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

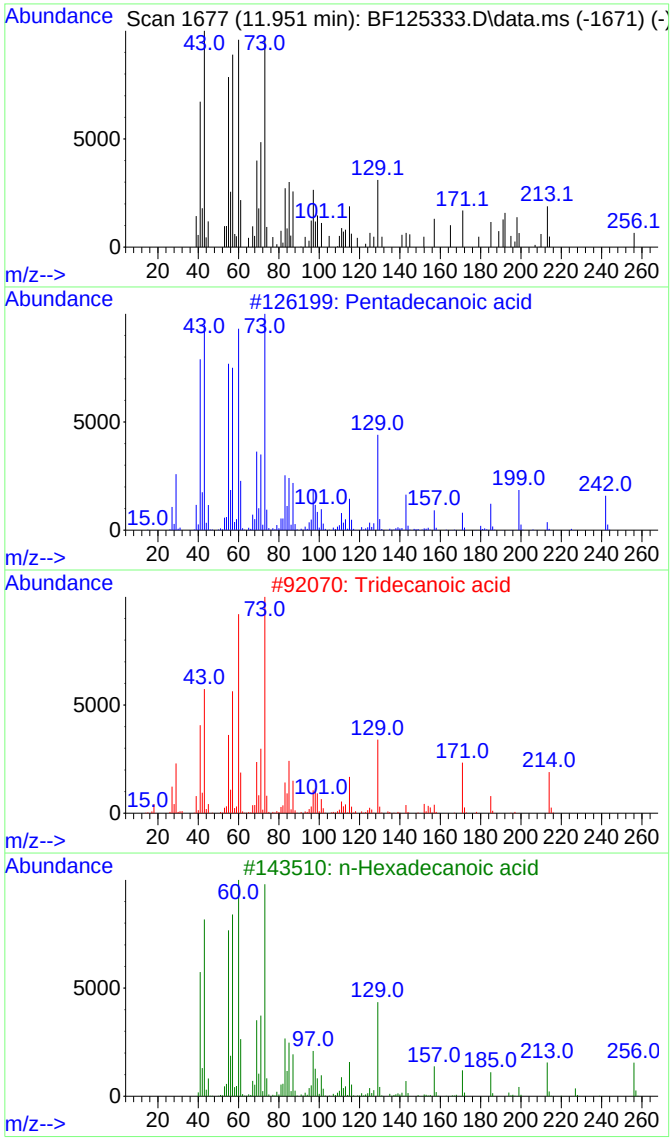
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

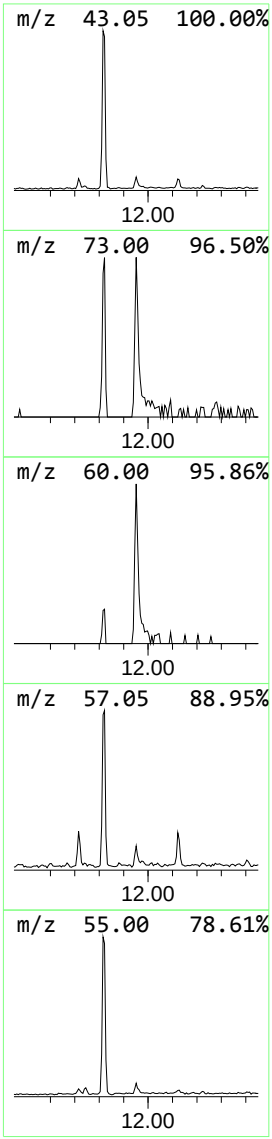
****

Peak Number 3 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.38 ng	164720	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
4	Tetradecane	198	C14H30	000629-59-4	25
5	Oxalic acid, allyl undecyl ester	284	C16H28O4	1000309-23-9	18





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Operator : JU/CG
Sample : M3636-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-090121

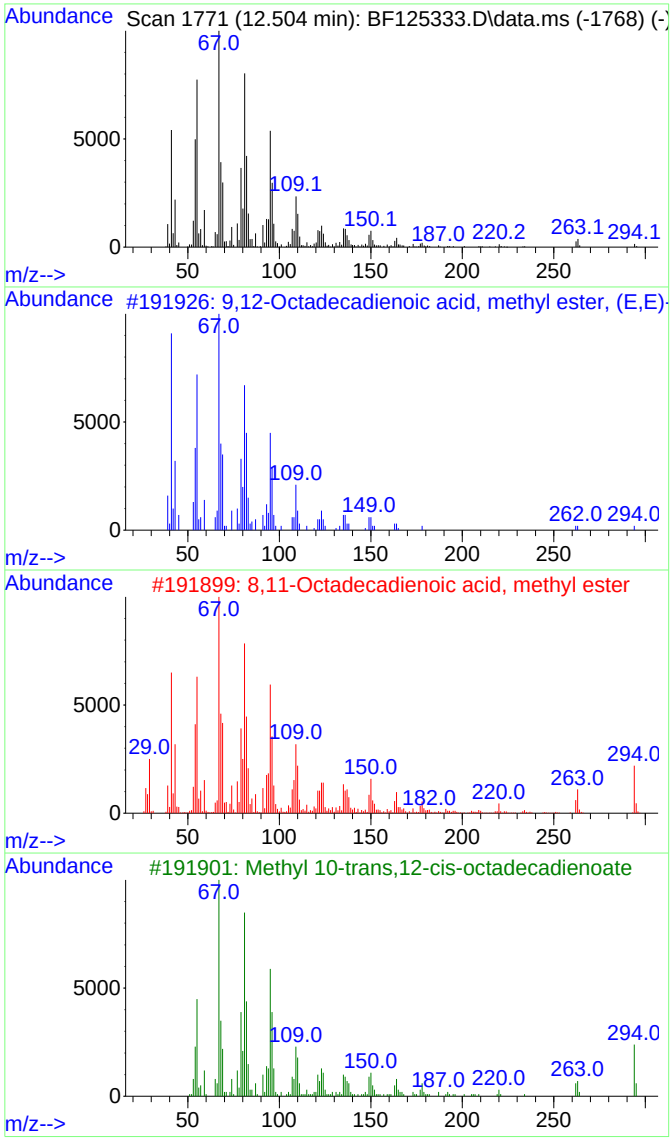
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

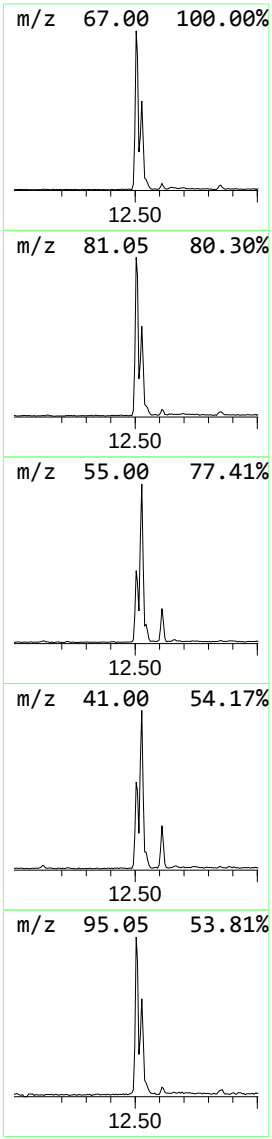
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.504	16.87 ng	1167680	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
2	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	97
3	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	95
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	94
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	94





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Instrument : BNA_F
ClientSampleId : SA-01-090121

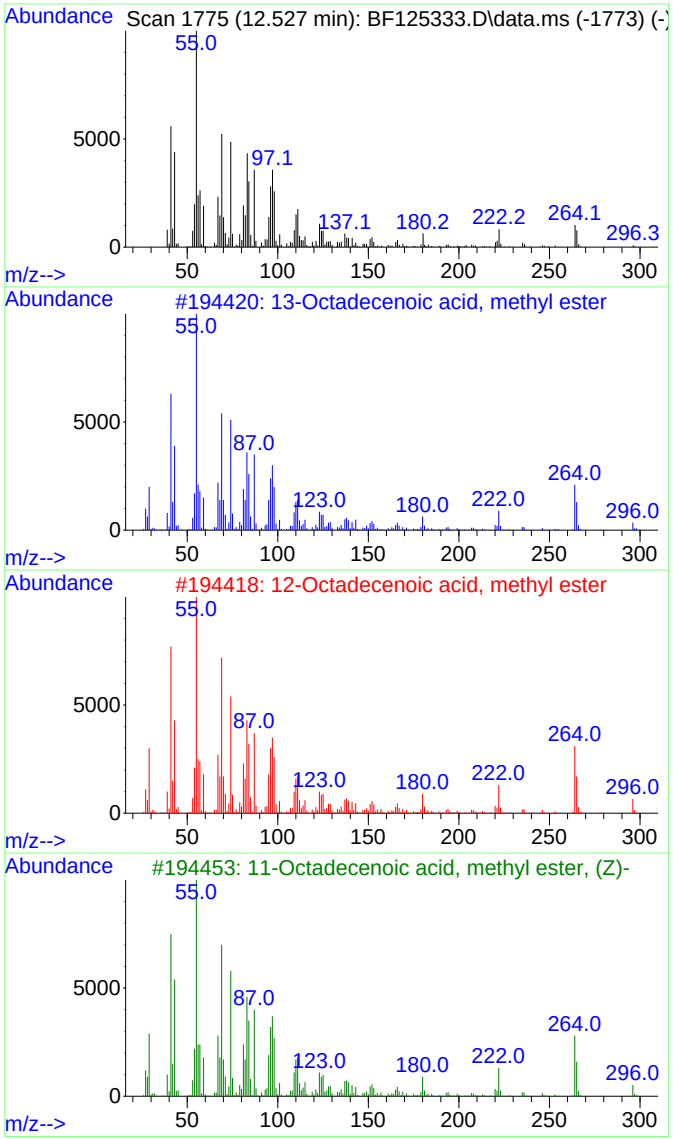
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

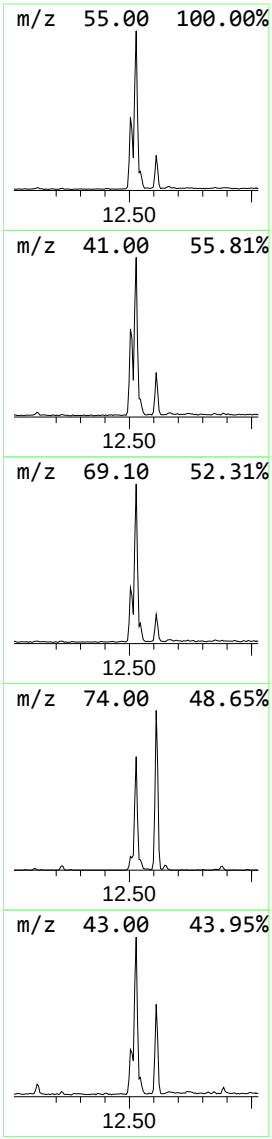
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 13-Octadecenoic acid, methy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	26.19 ng	1812940	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99





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Misc :
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Instrument : BNA_F
ClientSampleId : SA-01-090121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

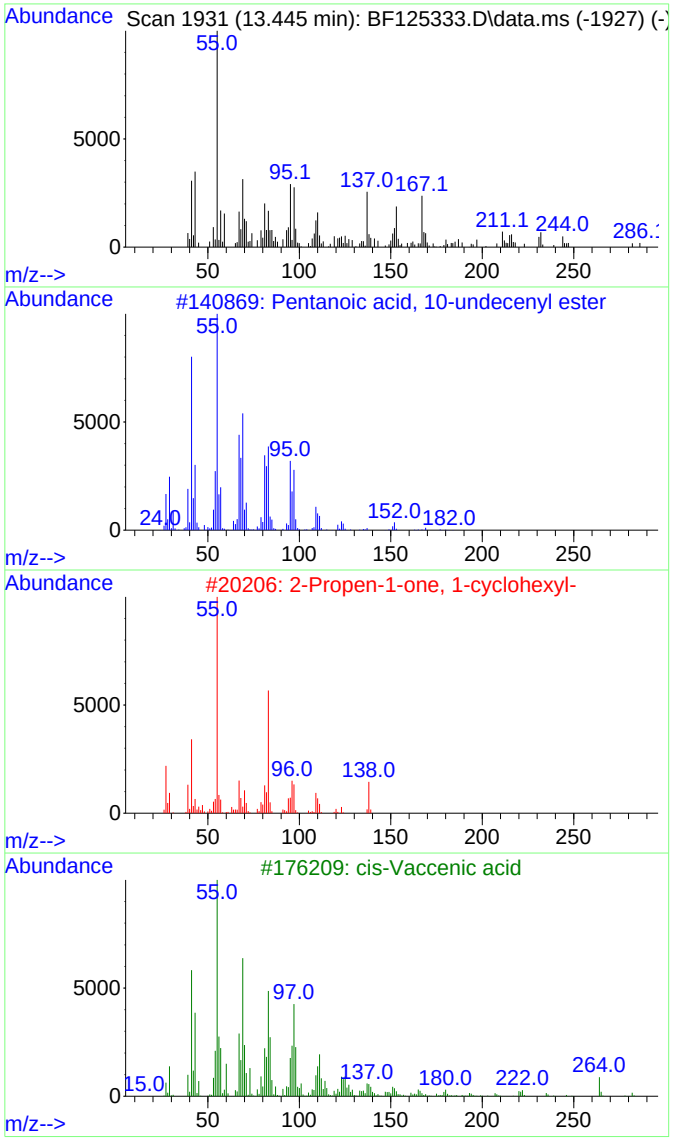
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

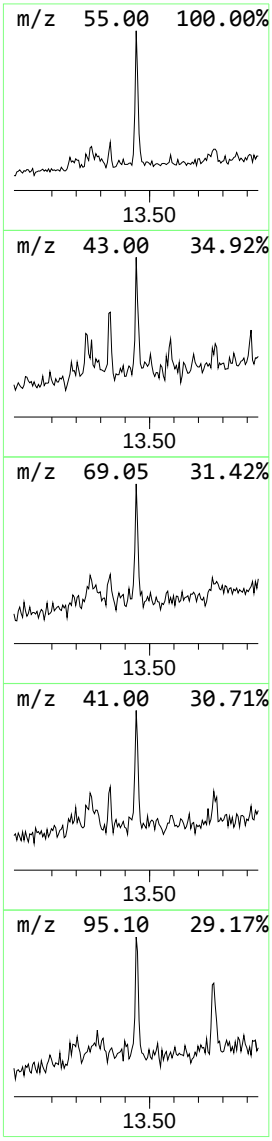
****

Peak Number 6 unknown13.445 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	2.78 ng	179317	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 10-undecenyl ester	254	C16H30O2	1000159-93-4	27
2	2-Propen-1-one, 1-cyclohexyl-	138	C9H14O	002177-34-6	14
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	12
4	Fumaric acid, di(2-methylallyl) ...	224	C12H16O4	1000330-55-8	10
5	Bicyclo[2.2.2]octane-2,6-dione	138	C8H10O2	038231-60-6	10





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SA-01-090121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

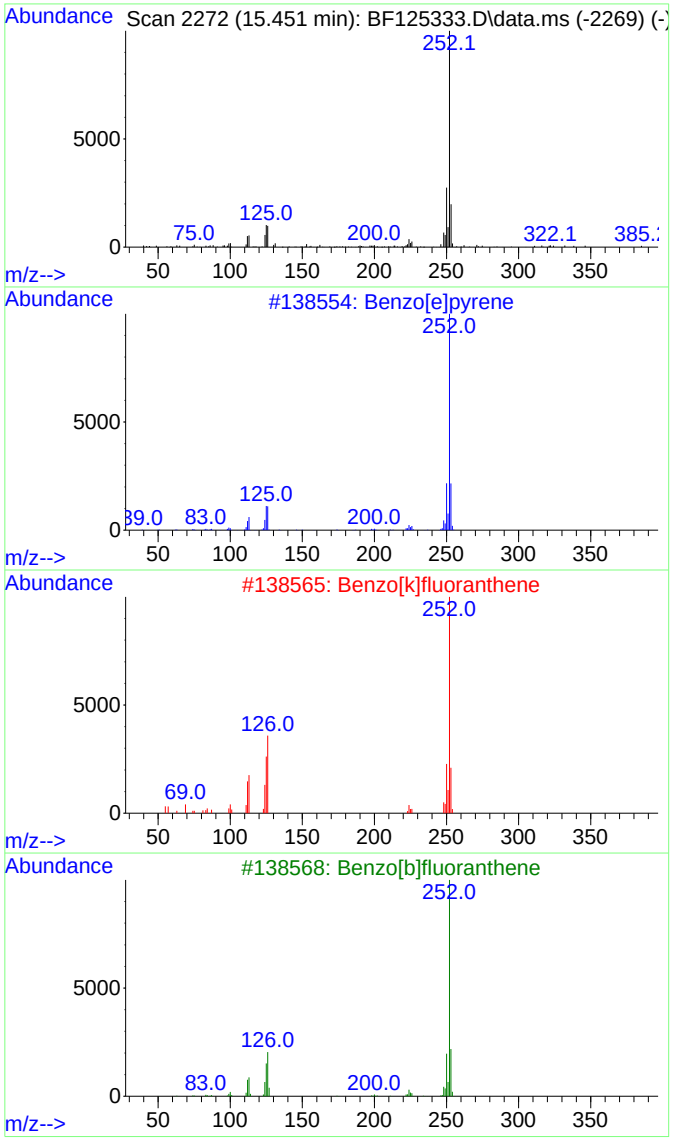
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

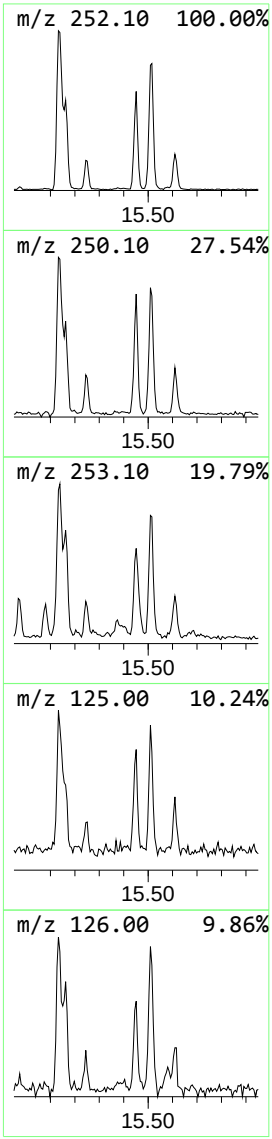
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.451	3.01 ng	161066	Perylene-d12	15.580

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090221\
Data File : BF125333.D
Acq On : 2 Sep 2021 21:48
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Misc :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.152	5.4	ng	259500	1	6.904	963766	20.0
Hexadecanoic ac...	11.822	16.7	ng	1154450	4	11.433	1384210	20.0
Pentadecanoic acid	11.951	2.4	ng	164720	4	11.433	1384210	20.0
9,12-Octadecadi...	12.504	16.9	ng	1167680	4	11.433	1384210	20.0
13-Octadecenoic...	12.527	26.2	ng	1812940	4	11.433	1384210	20.0
unknown13.445	13.445	2.8	ng	179317	5	14.080	1289270	20.0
Benzo[e]pyrene	15.451	3.0	ng	161066	6	15.580	1070240	20.0