LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122332.D
Acq On : 13 Nov 2020 16:41
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	19	rVB	943153	1294133	21.22%	2.472%
2	3.299	204	206	219	rBV	31898	73605	1.21%	0.141%
3	5.475	570	576	579	rBV	5233405	5039352	82.63%	9.626%
4	6.481	742	747	750	rBV	5055048	5234632	85.84%	9.999%
5	6.687	779	782	790	rBV	190846	168949	2.77%	0.323%
6	6.863	809	812	816	rBV	1893704	1449276	23.76%	2.768%
7	7.422	902	907	910	rBV	3561006	3367532	55.22%	6.432%
8	8.145	1027	1030	1034	rBV	2101425	1884179	30.90%	3.599%
9	9.228	1209	1214	1217	rBV	6481989	5754816	94.37%	10.992%
10	9.345	1231	1234	1237	rVB	328985	304088	4.99%	0.581%
11	9.616	1276	1280	1283	rBV	1383433	1045476	17.14%	1.997%
12	9.904	1325	1329	1332	rBV	2613286	2142385	35.13%	4.092%
13	10.686	1458	1462	1466	rBV	3755249	3361555	55.12%	6.421%
14	11.386	1577	1581	1583	rBV	2631024	2156435	35.36%	4.119%
15	11.410	1583	1585	1588	rVV	550012	408535	6.70%	0.780%
16	11.457	1591	1593	1597	rVB	106750	101349	1.66%	0.194%
17	11.886	1662	1666	1668	rBV	65337	64965	1.07%	0.124%
18	11.921	1668	1672	1676	rBV2	1061371	1074799	17.62%	2.053%
19	11.998	1682	1685	1688	rBV	92643	84303	1.38%	0.161%
20	12.174	1712	1715	1718	rBV2	65166	89726	1.47%	0.171%
21	12.204	1718	1720	1726	rVB2	58450	72079	1.18%	0.138%
22	12.374	1745	1749	1755	rVB	219810	200352	3.29%	0.383%
23	12.433	1755	1759	1763	rBV3	70576	119256	1.96%	0.228%
24	12.468	1763	1765	1771	rVB4	50271	81279	1.33%	0.155%
25	12.598	1783	1787	1790	rBV	921690	738315	12.11%	1.410%
26	12.639	1790	1794	1801	rVB5	69429	91930	1.51%	0.176%
27	12.704	1801	1805	1816	rBV2	847513	1439876	23.61%	2.750%
28	12.827	1820	1826	1829	rVB	699523	685807	11.25%	1.310%
29	12.974	1847	1851	1855	rVV	6298597	6098463	100.00%	11.649%
30	13.045	1859	1863	1866	rBV2	40634	63608	1.04%	0.121%
31	13.157	1879	1882	1885	rVB	94740	93892	1.54%	0.179%
32	13.221	1888	1893	1896	rVV3	78337	98425	1.61%	0.188%
33	13.257	1896	1899	1903	rBV	74223	76901	1.26%	0.147%
34	13.657	1964	1967	1973	rVB	61172	75382	1.24%	0.144%
35	13.774	1982	1987	1990	rBV2	71868	113041	1.85%	0.216%
36	13.880	2000	2005	2014	rBV2	415923	692042	11.35%	1.322%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122332.D
Acq On : 13 Nov 2020 16:41
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.027	2025	2030	2032	rBV2	2169931	2343673	38.43%	4.477%
38	14.051	2032	2034	2040	rVB	341818	293624	4.81%	0.561%
39	14.504	2105	2111	2113	rBV4	76267	115552	1.89%	0.221%
40	14.892	2173	2177	2183	rBV3	128393	155554	2.55%	0.297%
41	15.062	2202	2206	2209	rBV	280947	430420	7.06%	0.822%
42	15.157	2219	2222	2227	rVB2	57913	92038	1.51%	0.176%
43	15.368	2254	2258	2263	rVB	179427	230821	3.78%	0.441%
44	15.427	2264	2268	2273	rBV	221785	264747	4.34%	0.506%
45	15.492	2274	2279	2283	rBV	1647395	2009635	32.95%	3.839%
46	15.980	2358	2362	2367	rBV2	53895	79952	1.31%	0.153%
47	16.045	2369	2373	2381	rVV9	45766	107689	1.77%	0.206%
48	16.945	2521	2526	2535	rVB2	107021	233860	3.83%	0.447%
49	17.380	2596	2600	2606	rVB	84955	154168	2.53%	0.294%

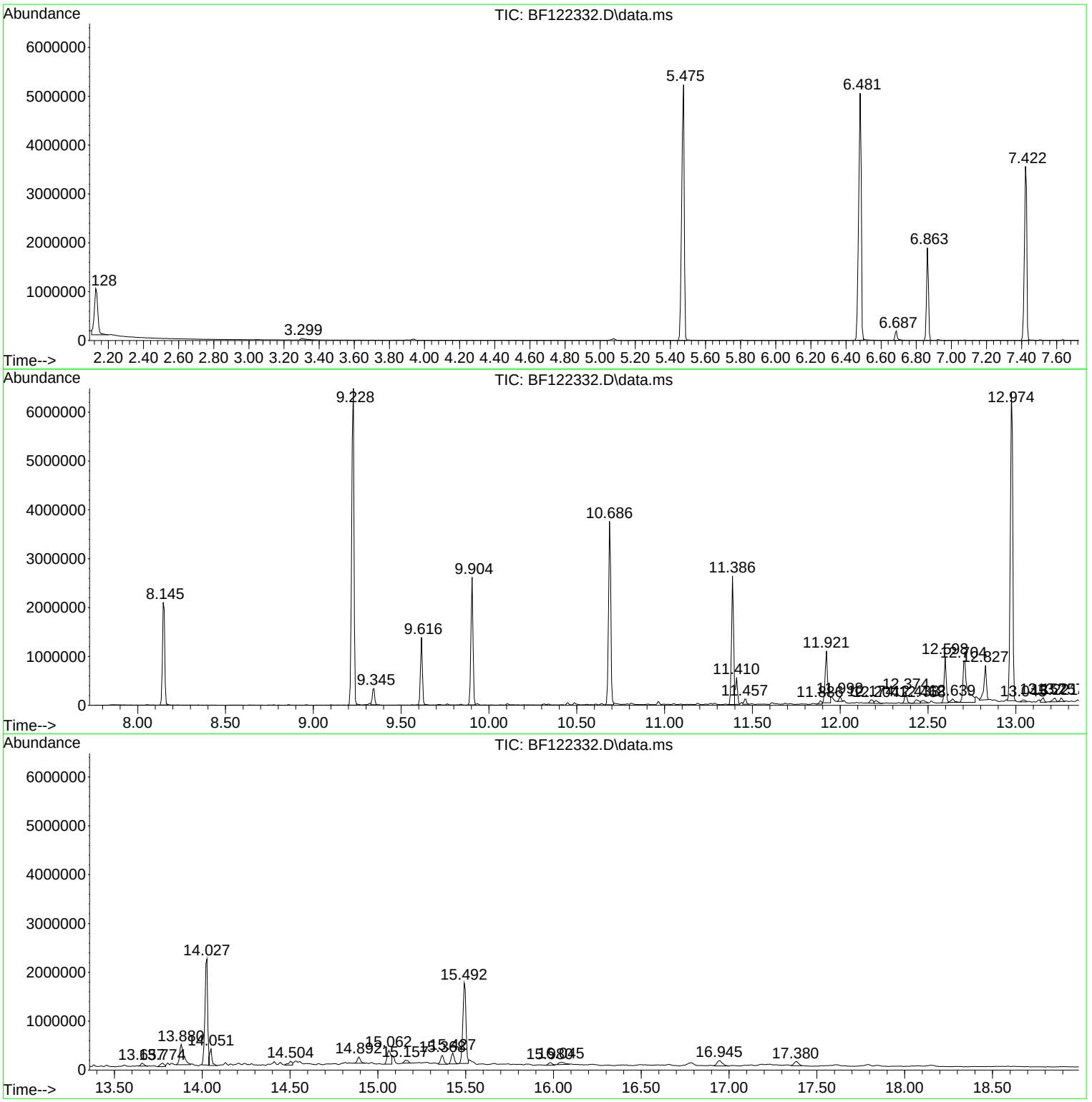
Sum of corrected areas: 52352471

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122332.D
Acq On : 13 Nov 2020 16:41
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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\BF111320\
Data File : BF122332.D
Acq On : 13 Nov 2020 16:41
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

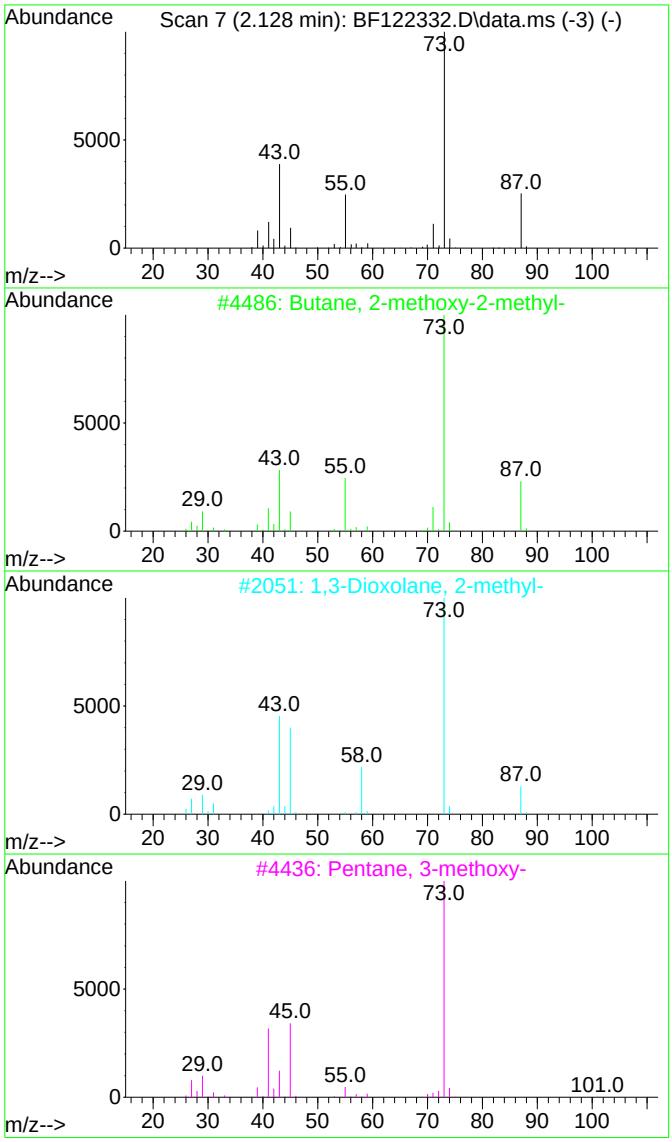
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

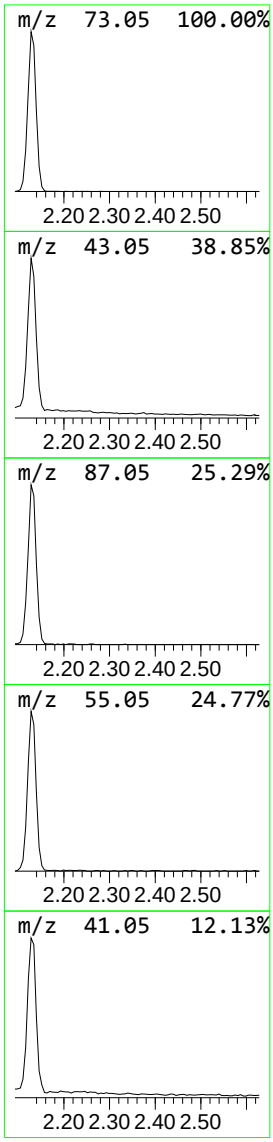
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	17.86 ng	1294130	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122332.D
Acq On : 13 Nov 2020 16:41
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

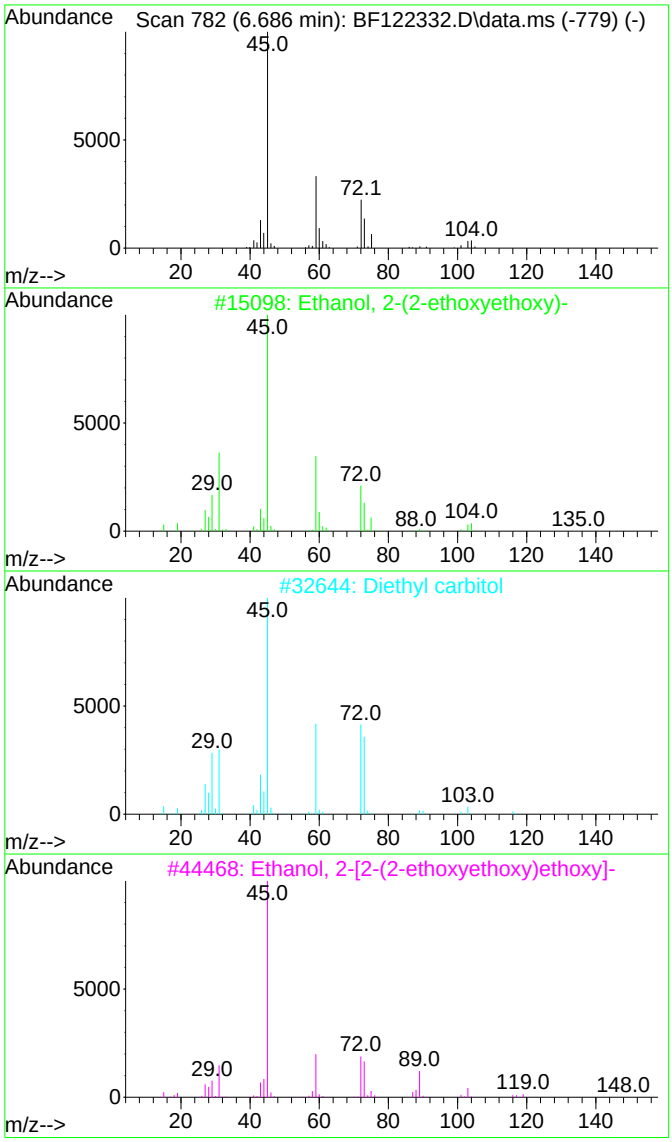
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

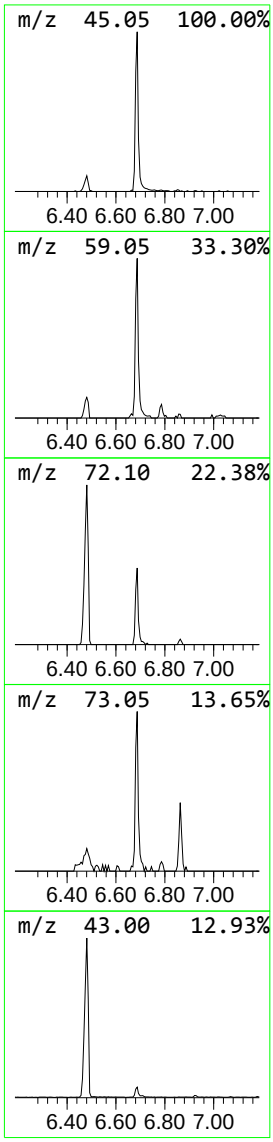
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.686	2.33 ng	168949	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5	Ethyl ether	74	C4H10O	000060-29-7	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122332.D
Acq On : 13 Nov 2020 16:41
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-31

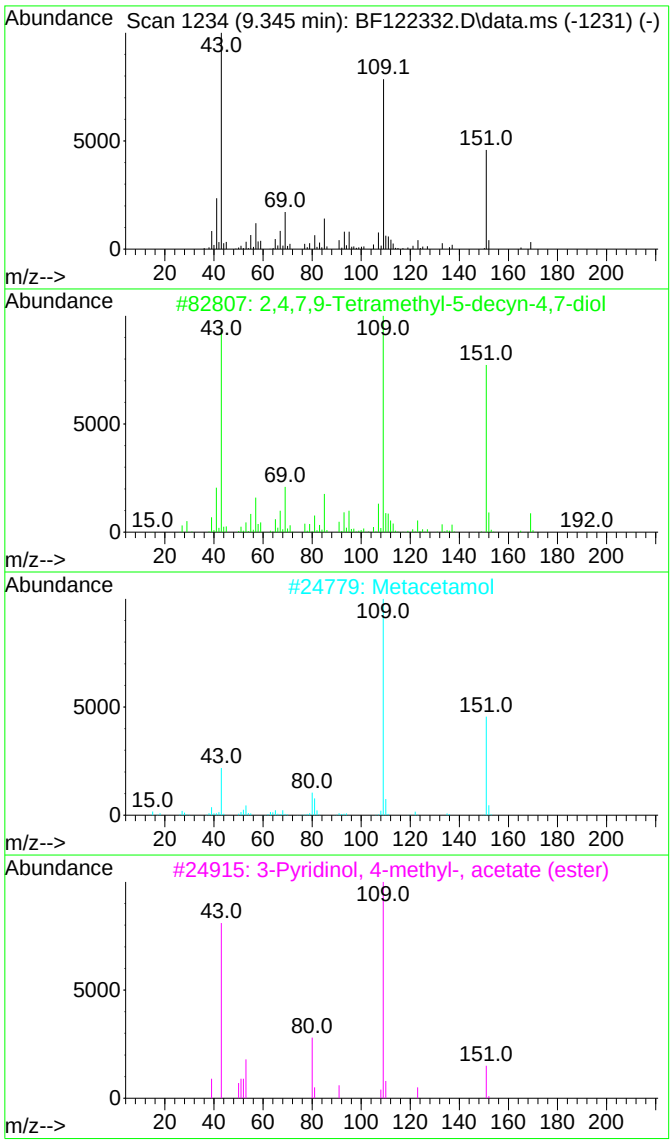
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

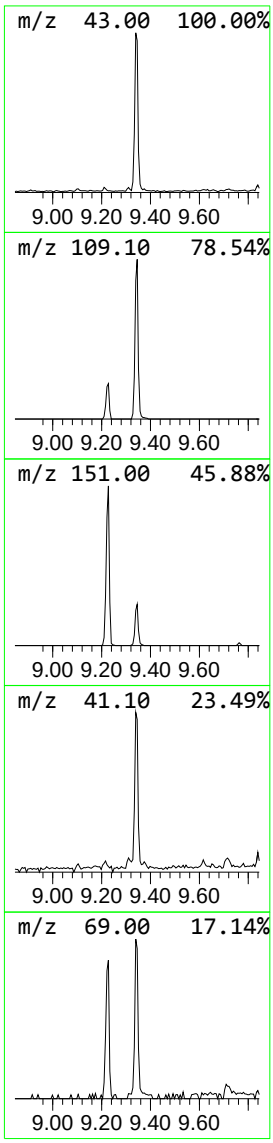
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.345	2.84 ng	304088	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	64
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59
5	Acetaminophen	151	C8H9NO2	000103-90-2	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122332.D
Acq On : 13 Nov 2020 16:41
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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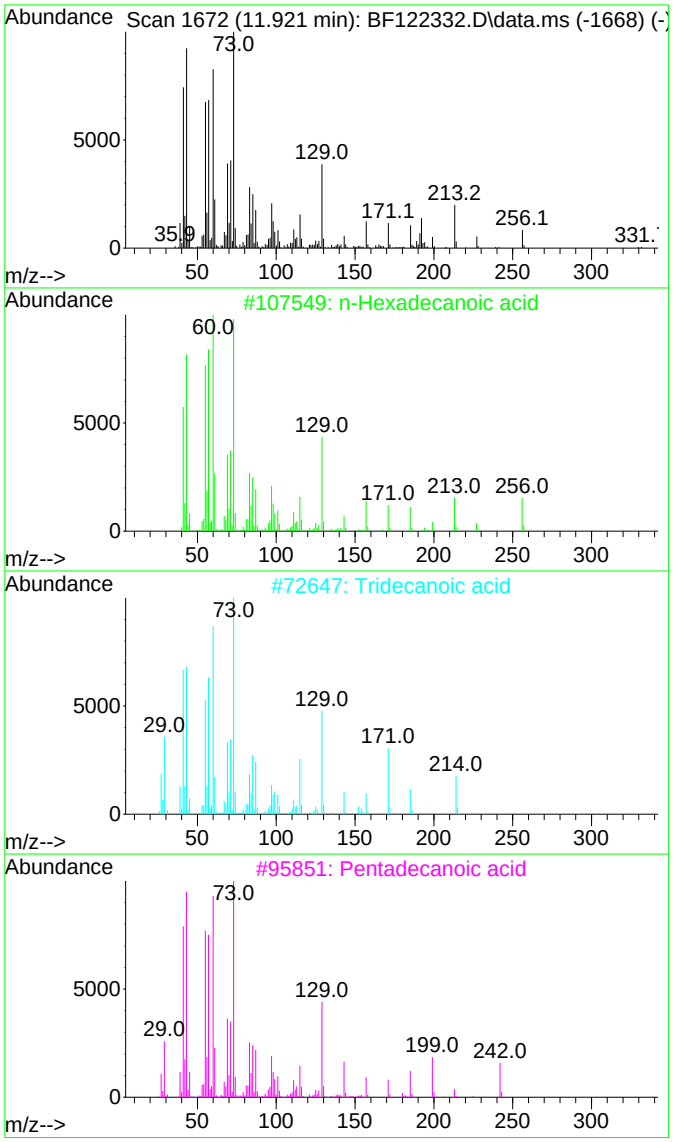
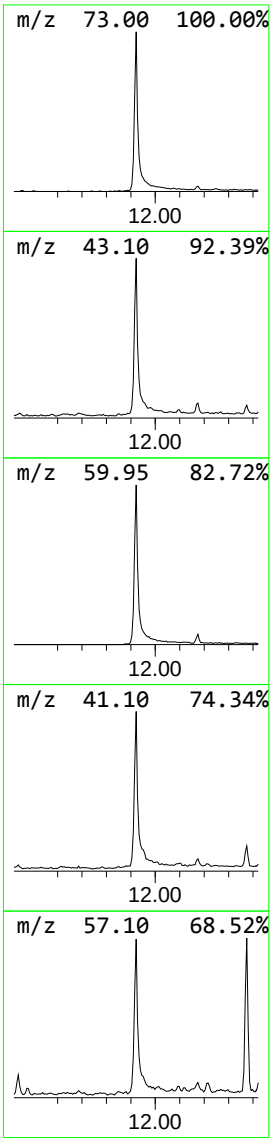
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	9.97 ng	1074800	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122332.D
Acq On : 13 Nov 2020 16:41
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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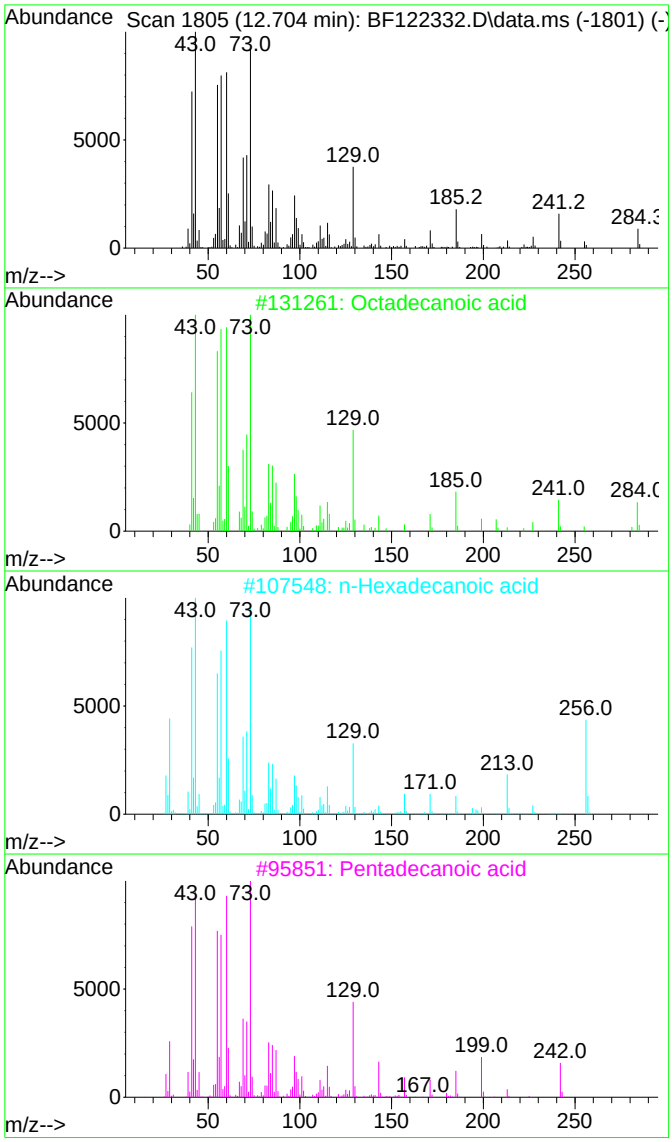
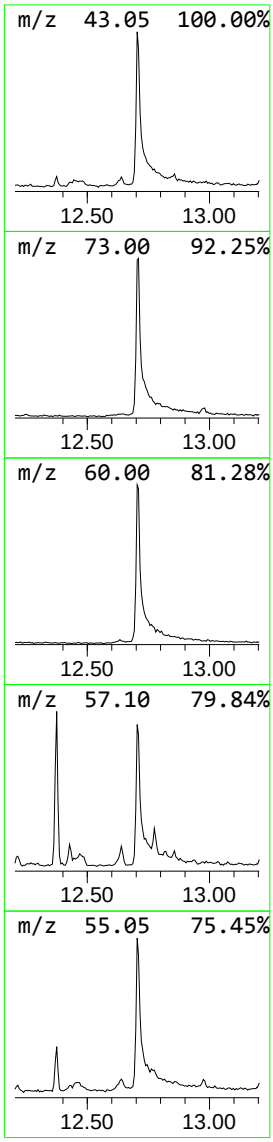
Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	13.35 ng	1439880	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122332.D
Acq On : 13 Nov 2020 16:41
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

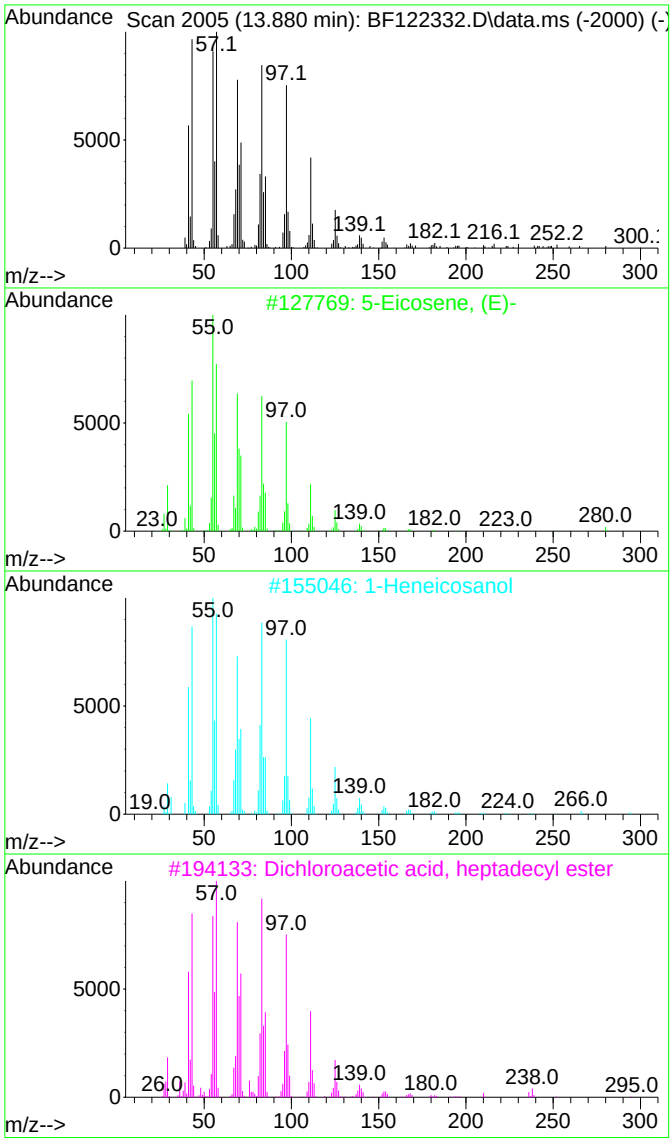
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

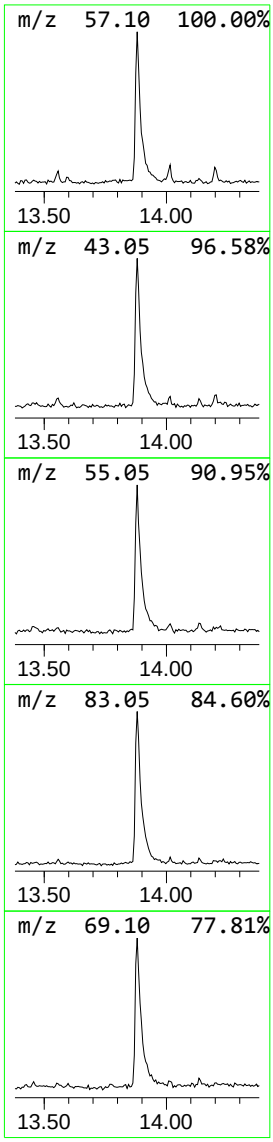
****

Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	5.91 ng	692042	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122332.D
Acq On : 13 Nov 2020 16:41
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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
Butane, 2-metho...	2.128	17.9	ng	1294130	1	6.863	1449280	20.0
Ethanol, 2-(2-e...	6.686	2.3	ng	168949	1	6.863	1449280	20.0
2,4,7,9-Tetrame...	9.345	2.8	ng	304088	3	9.904	2142390	20.0
n-Hexadecanoic ...	11.922	10.0	ng	1074800	4	11.386	2156440	20.0
Octadecanoic acid	12.704	13.4	ng	1439880	4	11.386	2156440	20.0
5-Eicosene, (E)-	13.880	5.9	ng	692042	5	14.027	2343670	20.0