LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
Data File : BF123452.D
Acq On : 24 Mar 2021 22:06
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-032321

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-BF032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123452.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	17	24	29	rVB	1052017	1325516	33.69%	4.047%
2	2.334	38	42	47	rVB2	70444	89414	2.27%	0.273%
3	5.140	510	519	524	rVB2	59964	87434	2.22%	0.267%
4	5.534	581	586	589	rBV	4220128	3915497	99.50%	11.954%
5	6.534	751	756	766	rBV	3603003	3935025	100.00%	12.014%
6	6.734	788	790	796	rBV	64486	65250	1.66%	0.199%
7	6.916	817	821	824	rBV	1475395	1150333	29.23%	3.512%
8	7.475	911	916	919	rBV	2826397	2439693	62.00%	7.449%
9	8.198	1034	1039	1042	rBV	1739554	1393378	35.41%	4.254%
10	8.881	1151	1155	1158	rBV	180180	214991	5.46%	0.656%
11	8.910	1158	1160	1165	rVB2	65890	62341	1.58%	0.190%
12	9.275	1218	1222	1225	rBV	4203841	3738909	95.02%	11.415%
13	9.357	1233	1236	1239	rBV2	38596	42239	1.07%	0.129%
14	9.392	1239	1242	1246	rVB	121136	98586	2.51%	0.301%
15	9.669	1286	1289	1293	rBV	178231	163560	4.16%	0.499%
16	9.957	1332	1338	1342	rBV	1587081	1305133	33.17%	3.985%
17	10.745	1468	1472	1476	rBV	2316013	1926705	48.96%	5.882%
18	11.163	1539	1543	1547	rBV	130936	130406	3.31%	0.398%
19	11.404	1581	1584	1588	rVB	61395	55144	1.40%	0.168%
20	11.451	1588	1592	1594	rBV	1315284	1118454	28.42%	3.415%
21	11.474	1594	1596	1598	rVV	147873	118413	3.01%	0.362%
22	11.522	1598	1604	1608	rVB2	49533	62827	1.60%	0.192%
23	11.663	1625	1628	1633	rBV2	95406	102074	2.59%	0.312%
24	11.845	1656	1659	1663	rVB	80701	64555	1.64%	0.197%
25	11.974	1679	1681	1686	rBV2	189748	164577	4.18%	0.502%
26	12.533	1773	1776	1778	rBV4	74022	83223	2.11%	0.254%
27	12.551	1778	1779	1782	rVB2	78660	65902	1.67%	0.201%
28	12.663	1796	1798	1802	rBV	405737	349771	8.89%	1.068%
29	12.892	1831	1837	1840	rBV	364688	421371	10.71%	1.286%
30	13.039	1858	1862	1866	rVB	3355963	3067811	77.96%	9.366%
31	13.116	1871	1875	1878	rBV5	27343	44297	1.13%	0.135%
32	13.227	1891	1894	1896	rVB	77116	61227	1.56%	0.187%
33	13.292	1903	1905	1907	rVB	68844	51826	1.32%	0.158%
34	13.945	2012	2016	2024	rVB	528492	584314	14.85%	1.784%
35	14.098	2037	2042	2045	rBV2	1378662	1512339	38.43%	4.617%
36	14.121	2045	2046	2052	rVB	279113	228541	5.81%	0.698%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032421\
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Acq On : 24 Mar 2021 22:06
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-032321

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-BF032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.204	2058	2060	2064	rBV	89437	85546	2.17%	0.261%
38	14.580	2121	2124	2128	rBV	250542	252152	6.41%	0.770%
39	15.162	2219	2223	2226	rBV	317039	480041	12.20%	1.466%
40	15.474	2273	2276	2283	rVB	219913	253399	6.44%	0.774%
41	15.539	2284	2287	2291	rVB	267935	306354	7.79%	0.935%
42	15.609	2294	2299	2302	rBV	738188	929083	23.61%	2.837%
43	17.127	2553	2557	2562	rBV	113478	206195	5.24%	0.630%

Sum of corrected areas: 32753846

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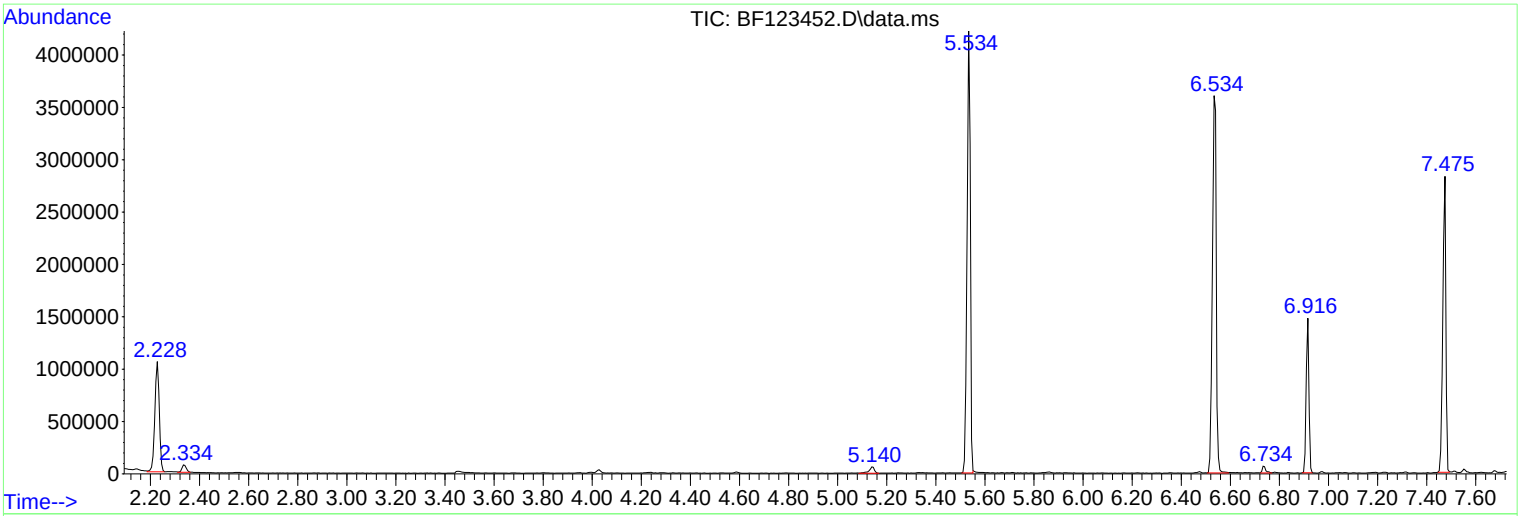
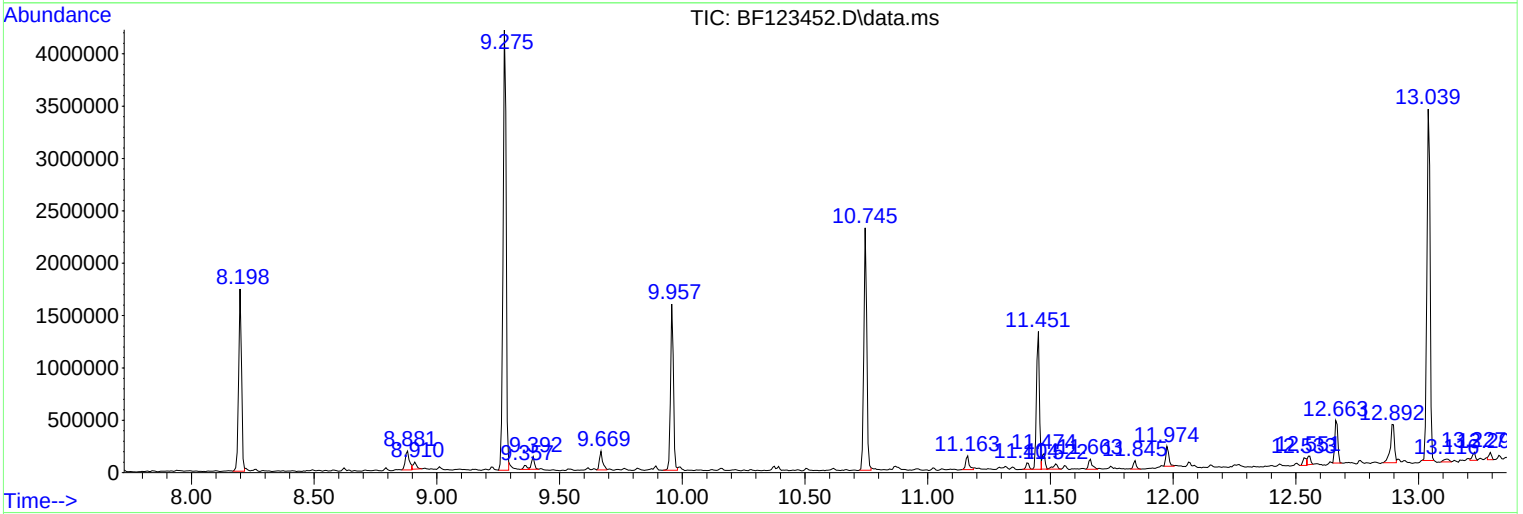
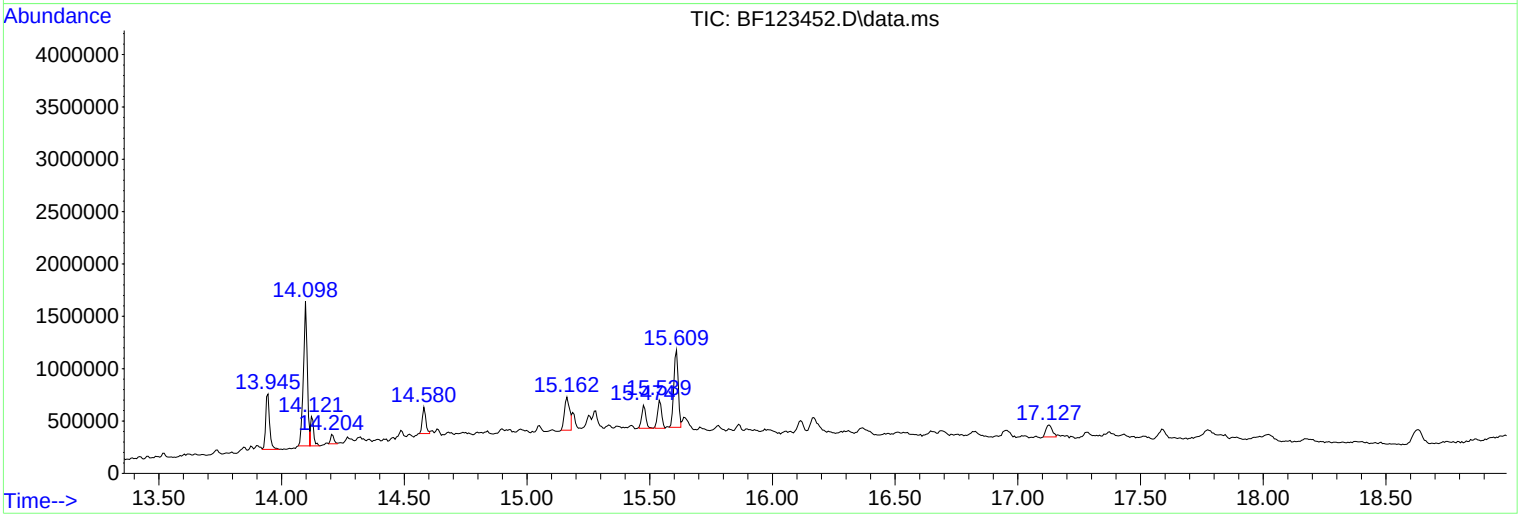
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Instrument : BNA_F
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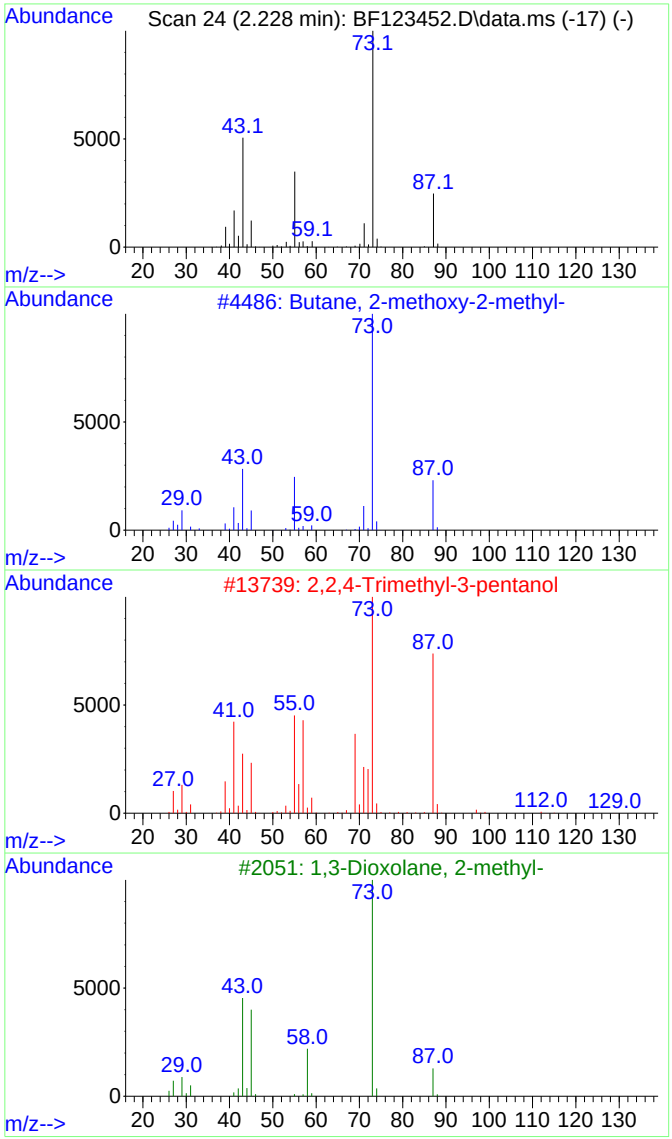
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

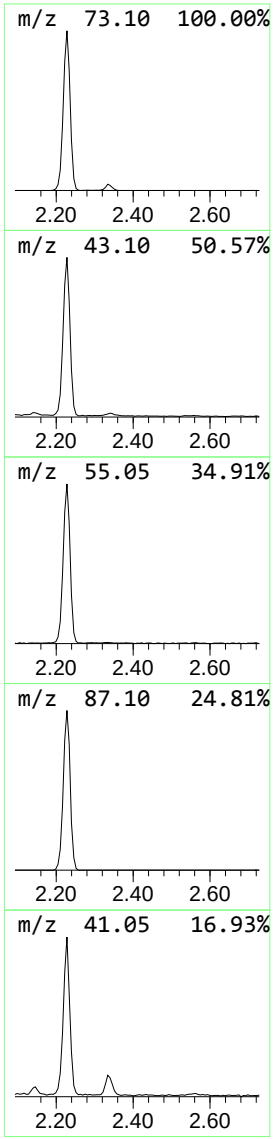
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	23.05 ng	1325520	1,4-Dichlorobenzene-d4	6.916

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

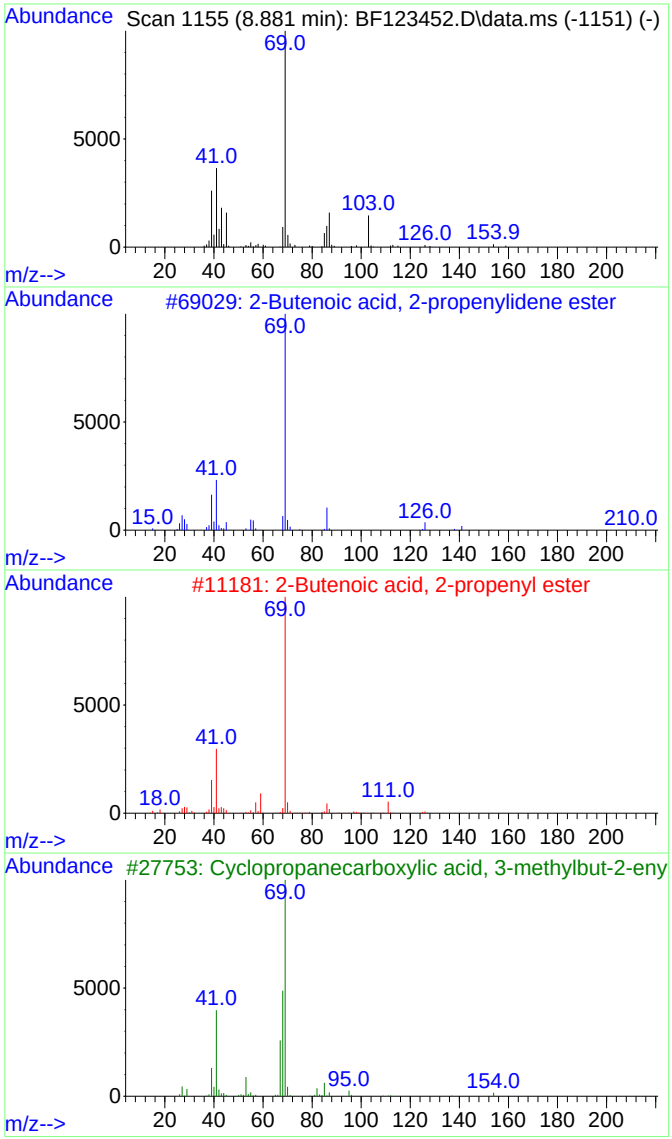
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

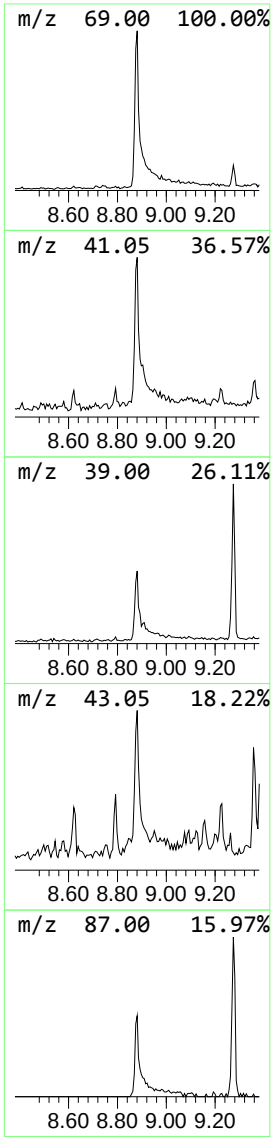
****

Peak Number 2 unknown8.881 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.881	3.09 ng	214991	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
2	2-Butenoic acid, 2-propenyl ester	126	C7H10O2	020474-93-5	40
3	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	38
4	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38
5	Cyclopropanecarboxylic acid, sil...	192	C4H5AgO2	075112-77-5	33





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Acq On : 24 Mar 2021 22:06
Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

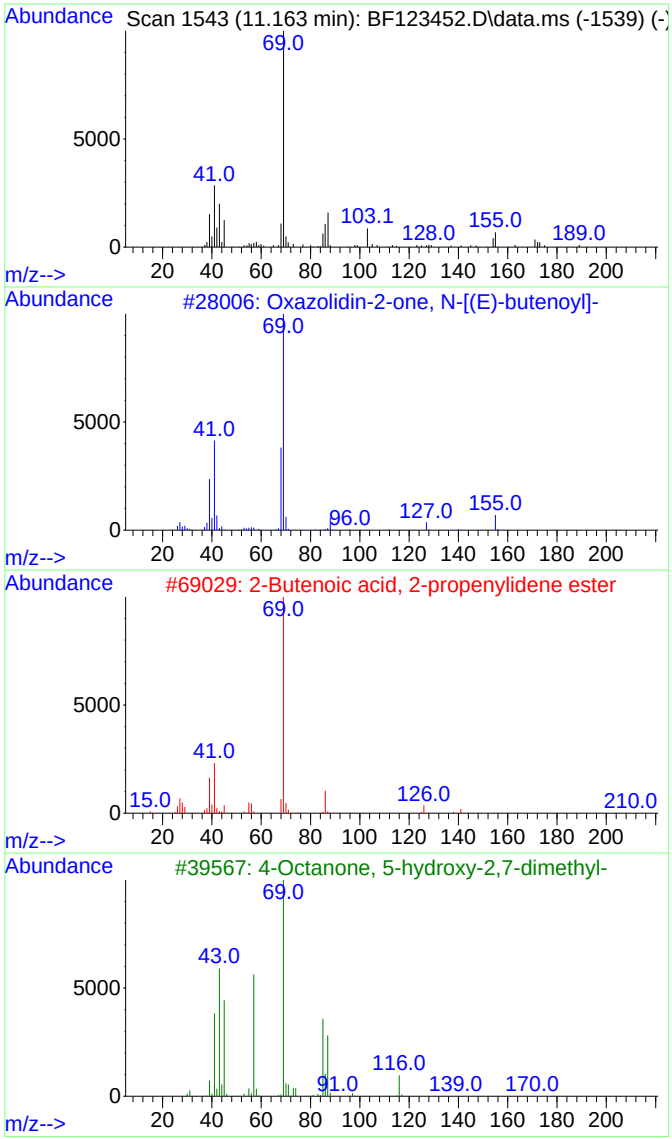
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

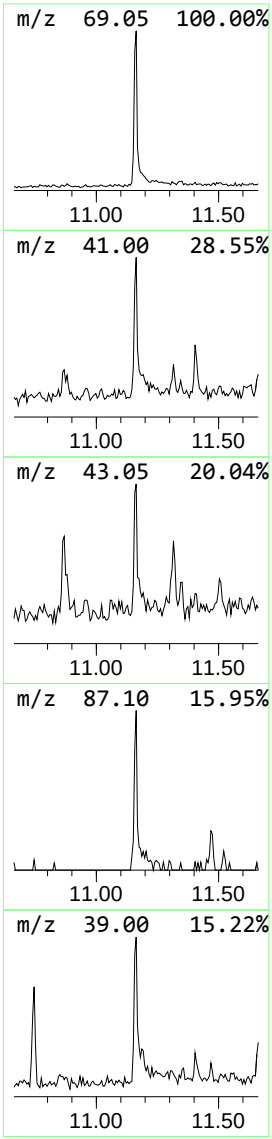
****

Peak Number 3 unknown11.163 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.163	2.33 ng	130406	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolidin-2-one, N-[(E)-butenoyl]-	155	C7H9NO3	1000156-45-5	47
2	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
3	4-Octanone, 5-hydroxy-2,7-dimethyl-	172	C10H20O2	006838-51-3	36
4	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	34
5	Cyclopropanecarboxylic acid, sil...	192	C4H5AgO2	075112-77-5	33





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Operator : JU/CG
Sample : M1773-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

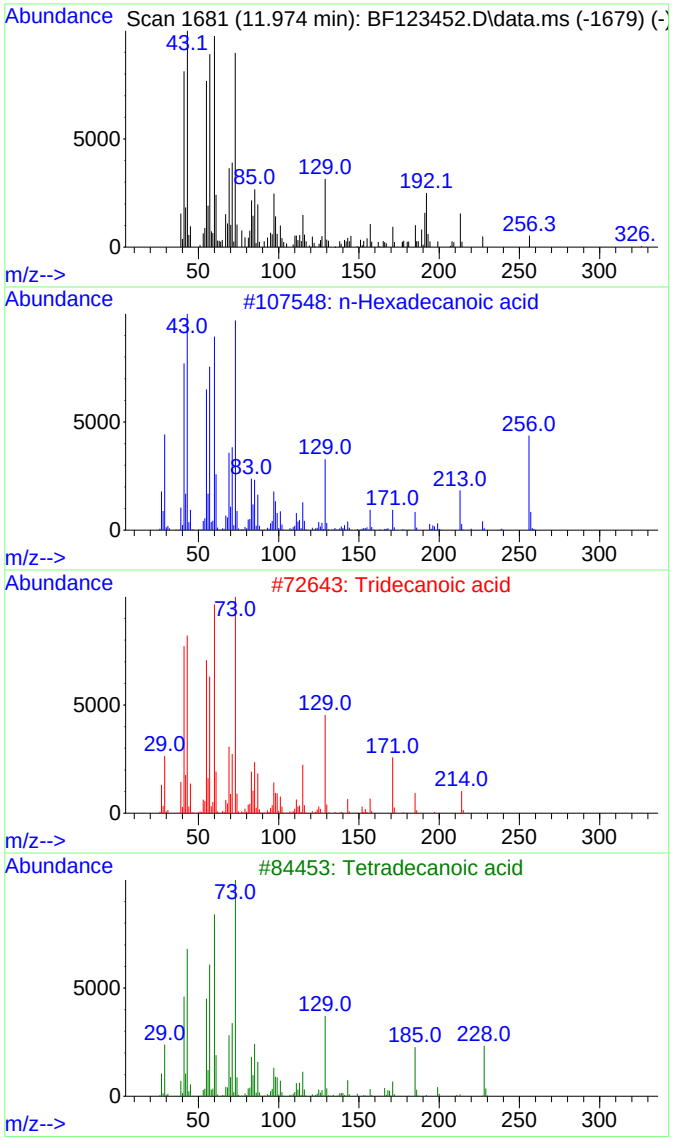
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

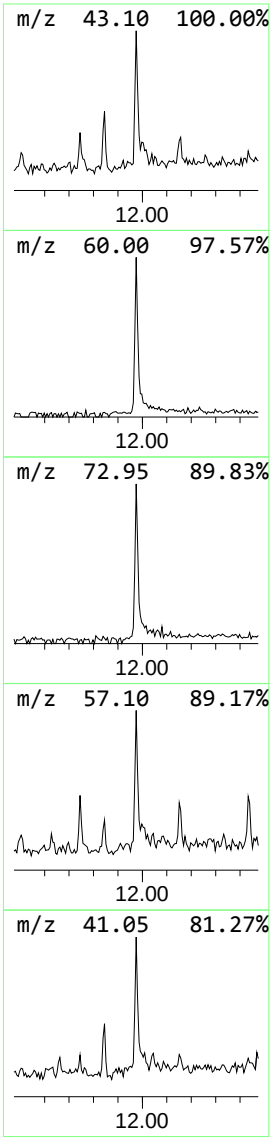
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.974	2.94 ng	164577	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	80
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	80





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Instrument :
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ClientSampleId :
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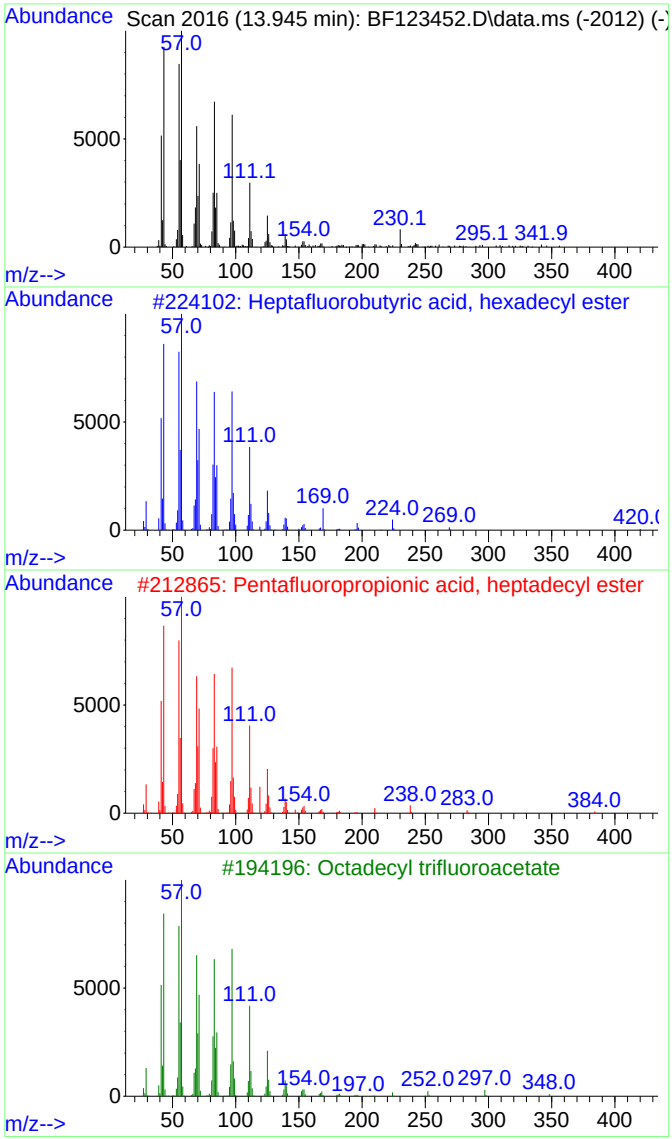
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

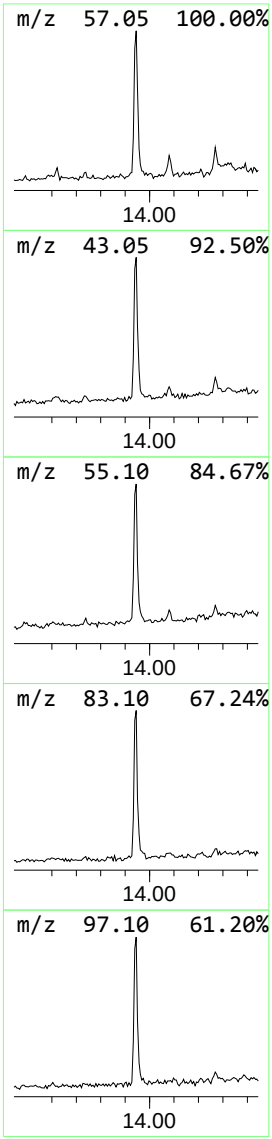
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	7.73 ng	584314	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-032321

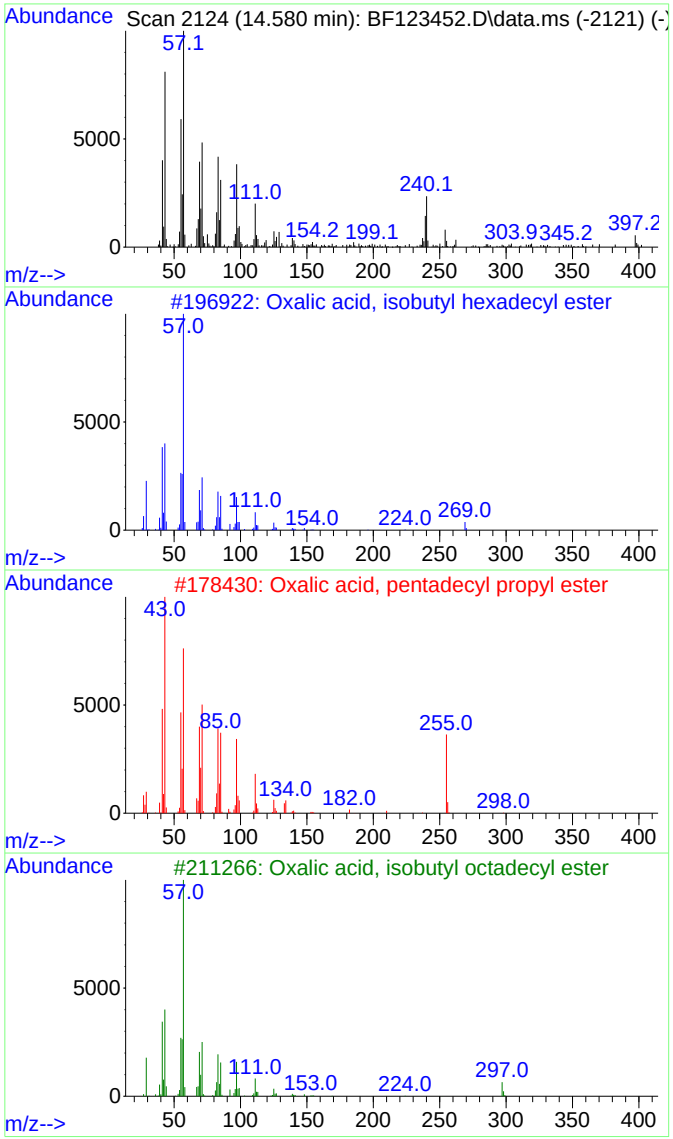
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

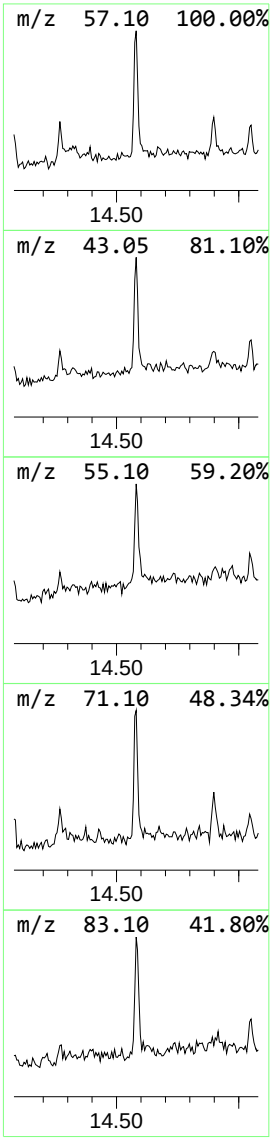
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Oxalic acid, isobutyl hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	3.33 ng	252152	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	81
2	Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	81
3	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	74
4	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	72
5	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	72





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

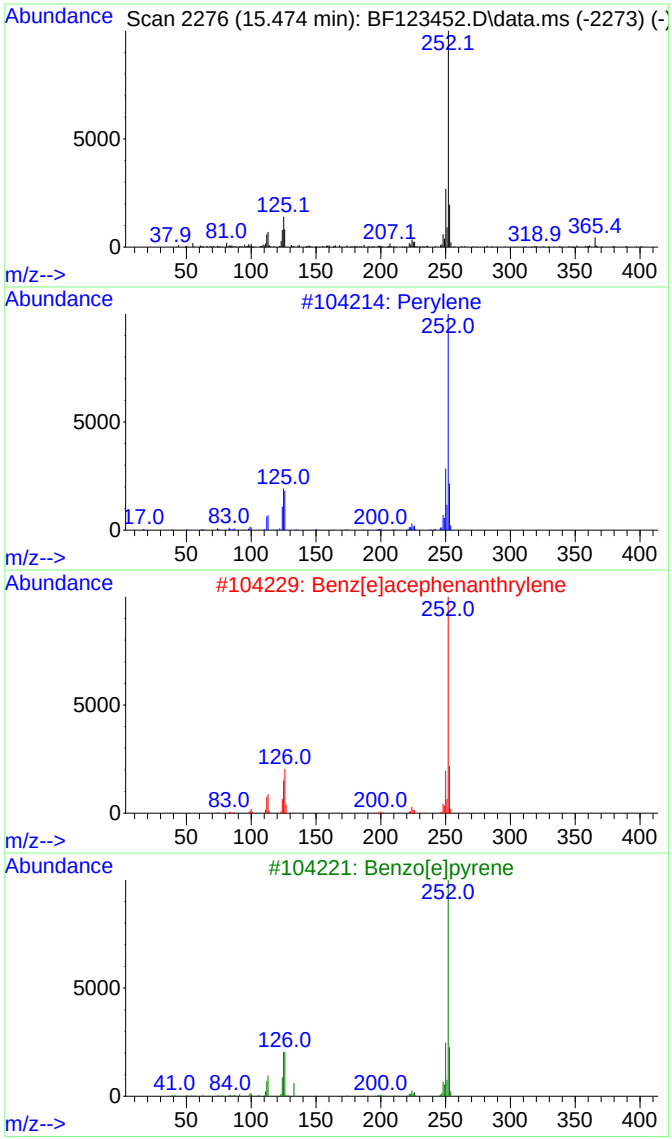
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

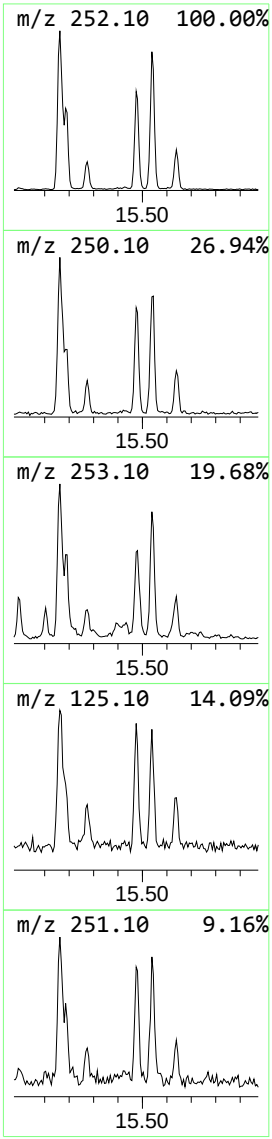
****

Peak Number 7 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.474	5.45 ng	253399	Perylene-d12	15.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
3	Benzo[e]pyrene	252	C20H12	000192-97-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Tentatively Identified Compound (LSC) summary

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-032321

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.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...	2.228	23.1	ng	1325520	1	6.916	1150330	20.0
unknown8.881	8.881	3.1	ng	214991	2	8.198	1393380	20.0
unknown11.163	11.163	2.3	ng	130406	4	11.451	1118450	20.0
n-Hexadecanoic ...	11.974	2.9	ng	164577	4	11.451	1118450	20.0
Heptafluorobuty...	13.945	7.7	ng	584314	5	14.098	1512340	20.0
Oxalic acid, is...	14.580	3.3	ng	252152	5	14.098	1512340	20.0
Perylene	15.474	5.5	ng	253399	6	15.610	929083	20.0