LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02

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: BF122454.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	15	rVB	524125	665099	18.30%	1.758%
2	2.246	23	27	33	rVB	50372	64578	1.78%	0.171%
3	4.451	398	402	407	rVB	65056	71474	1.97%	0.189%
4	5.075	502	508	520	rVB	1655823	1976535	54.40%	5.225%
5	5.487	573	578	581	rBV	3710772	3375798	92.91%	8.924%
6	5.875	641	644	649	rVB	212715	174807	4.81%	0.462%
7	6.492	744	749	767	rBV	3279769	3591374	98.84%	9.494%
8	6.692	780	783	788	rBV	60498	70805	1.95%	0.187%
9	6.863	808	812	815	rBV	1414680	1072154	29.51%	2.834%
10	7.422	903	907	911	rBV	2147332	2128775	58.59%	5.627%
11	8.151	1026	1031	1034	rBV	1526376	1336119	36.77%	3.532%
12	9.228	1209	1214	1217	rBV	4284539	3633589	100.00%	9.605%
13	9.310	1225	1228	1232	rBV4	85387	92490	2.55%	0.244%
14	9.622	1277	1281	1285	rBV	605991	562501	15.48%	1.487%
15	9.675	1288	1290	1295	rVB4	33875	46973	1.29%	0.124%
16	9.781	1303	1308	1310	rBV2	69857	106218	2.92%	0.281%
17	9.822	1312	1315	1317	rBV	94999	74216	2.04%	0.196%
18	9.910	1323	1330	1333	rBV	1584224	1514050	41.67%	4.002%
19	10.110	1361	1364	1371	rVB5	29988	47656	1.31%	0.126%
20	10.339	1401	1403	1406	rVB	122880	102030	2.81%	0.270%
21	10.451	1419	1422	1428	rBV3	47110	67133	1.85%	0.177%
22	10.563	1436	1441	1447	rVV2	122841	170107	4.68%	0.450%
23	10.616	1447	1450	1453	rVB4	41089	44530	1.23%	0.118%
24	10.698	1459	1464	1472	rBV	2428615	2404310	66.17%	6.356%
25	10.816	1481	1484	1485	rBV	184786	153854	4.23%	0.407%
26	11.033	1519	1521	1524	rBV3	42714	49395	1.36%	0.131%
27	11.263	1557	1560	1563	rBV	134975	128106	3.53%	0.339%
28	11.298	1563	1566	1571	rVB	130262	146245	4.02%	0.387%
29	11.398	1579	1583	1585	rBV	1470957	1345398	37.03%	3.557%
30	11.422	1585	1587	1590	rVV	373678	311613	8.58%	0.824%
31	11.469	1593	1595	1598	rVB	105820	88288	2.43%	0.233%
32	11.692	1630	1633	1636	rVB	136550	100874	2.78%	0.267%
33	11.927	1670	1673	1677	rBV2	248501	228611	6.29%	0.604%
34	12.010	1684	1687	1690	rBV	88037	91517	2.52%	0.242%
35	12.104	1700	1703	1705	rBV	92104	72731	2.00%	0.192%
36	12.451	1760	1762	1765	rBV	56800	55999	1.54%	0.148%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02

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	12.492	1766	1769	1774	rVB2	95789	94922	2.61%	0.251%
38	12.533	1774	1776	1781	rBV	59837	70071	1.93%	0.185%
39	12.616	1786	1790	1793	rBV	849093	711894	19.59%	1.882%
40	12.710	1803	1806	1811	rBV5	84681	118347	3.26%	0.313%
41	12.839	1823	1828	1831	rBV	765077	745396	20.51%	1.970%
42	12.986	1849	1853	1856	rBV	3776021	3191091	87.82%	8.436%
43	13.057	1863	1865	1869	rVB	51401	60028	1.65%	0.159%
44	13.169	1882	1884	1887	rVB2	85733	70633	1.94%	0.187%
45	13.239	1891	1896	1898	rVV2	51546	67800	1.87%	0.179%
46	13.274	1899	1902	1905	rVV	75404	78086	2.15%	0.206%
47	13.398	1921	1923	1926	rBV	50659	56479	1.55%	0.149%
48	13.674	1968	1970	1976	rVB	64384	73586	2.03%	0.195%
49	13.792	1987	1990	1992	rBV2	48785	64433	1.77%	0.170%
50	13.821	1992	1995	1996	rBV	64664	58997	1.62%	0.156%
51	13.898	2005	2008	2016	rVB4	192922	308781	8.50%	0.816%
52	14.039	2028	2032	2035	rBV2	1378124	1611209	44.34%	4.259%
53	14.068	2035	2037	2043	rVB	340097	336074	9.25%	0.888%
54	14.145	2048	2050	2053	rVB	62172	51689	1.42%	0.137%
55	15.086	2206	2210	2219	rVB2	460757	984469	27.09%	2.602%
56	15.392	2259	2262	2268	rVB	255010	320555	8.82%	0.847%
57	15.457	2269	2273	2279	rVB	336928	432958	11.92%	1.145%
58	15.521	2279	2284	2288	rBV	1096725	1409459	38.79%	3.726%
59	16.992	2530	2534	2543	rVB2	193374	392681	10.81%	1.038%
60	17.433	2605	2609	2621	rVB	154266	353566	9.73%	0.935%

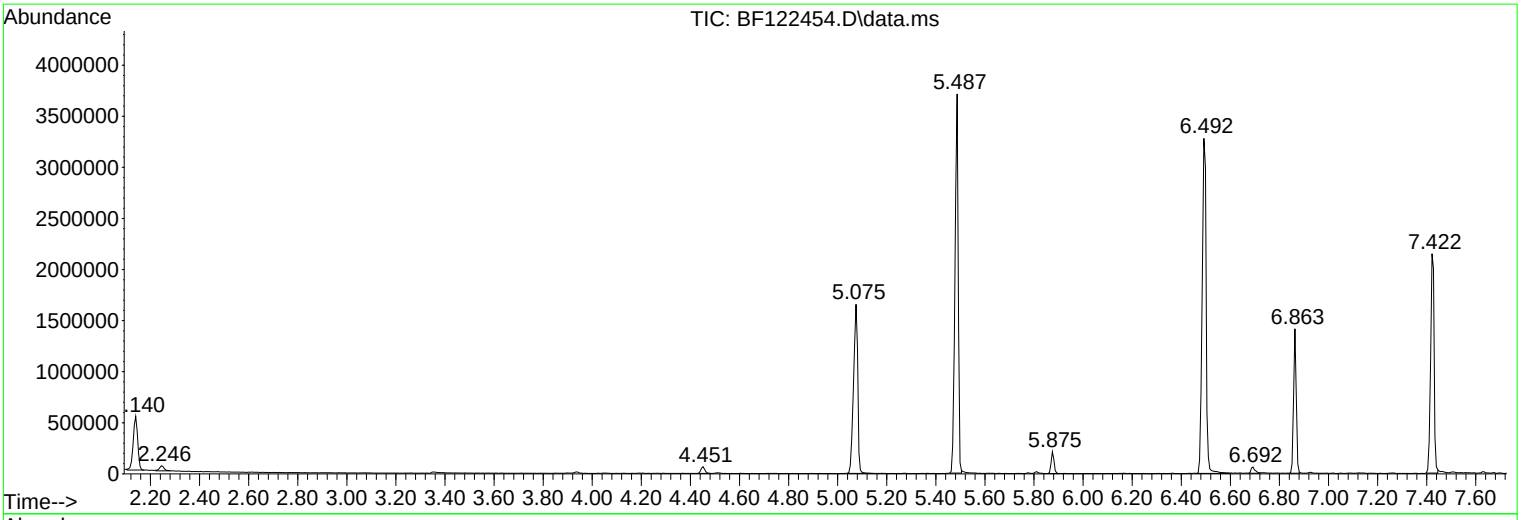
Sum of corrected areas: 37829156

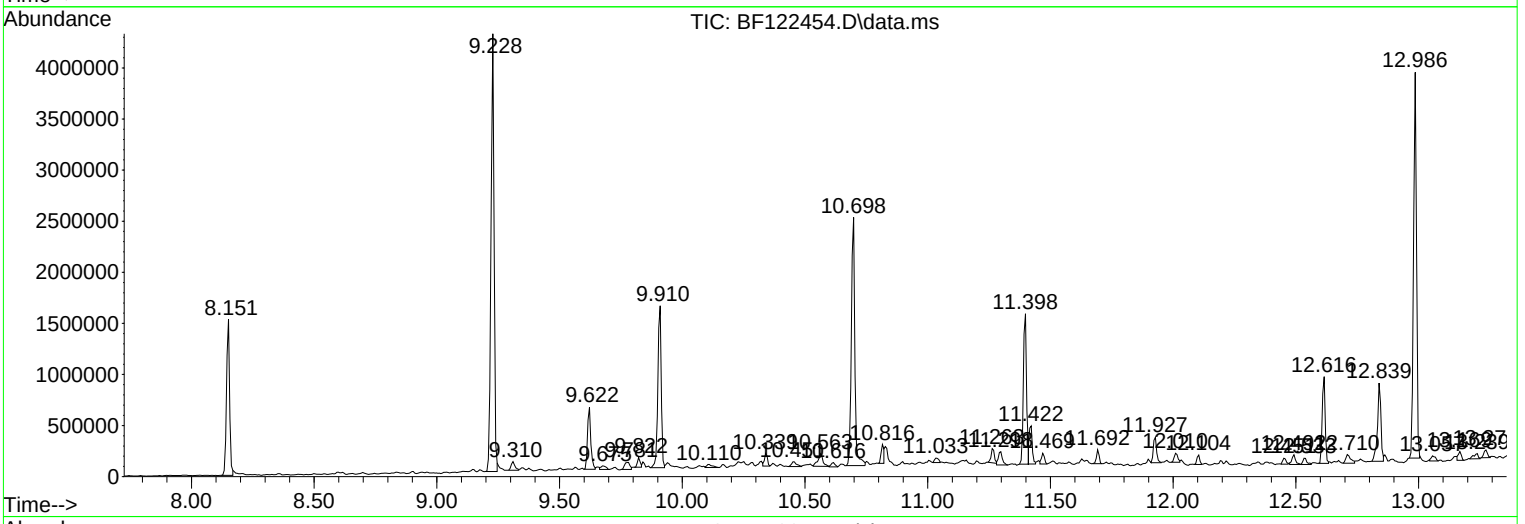
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

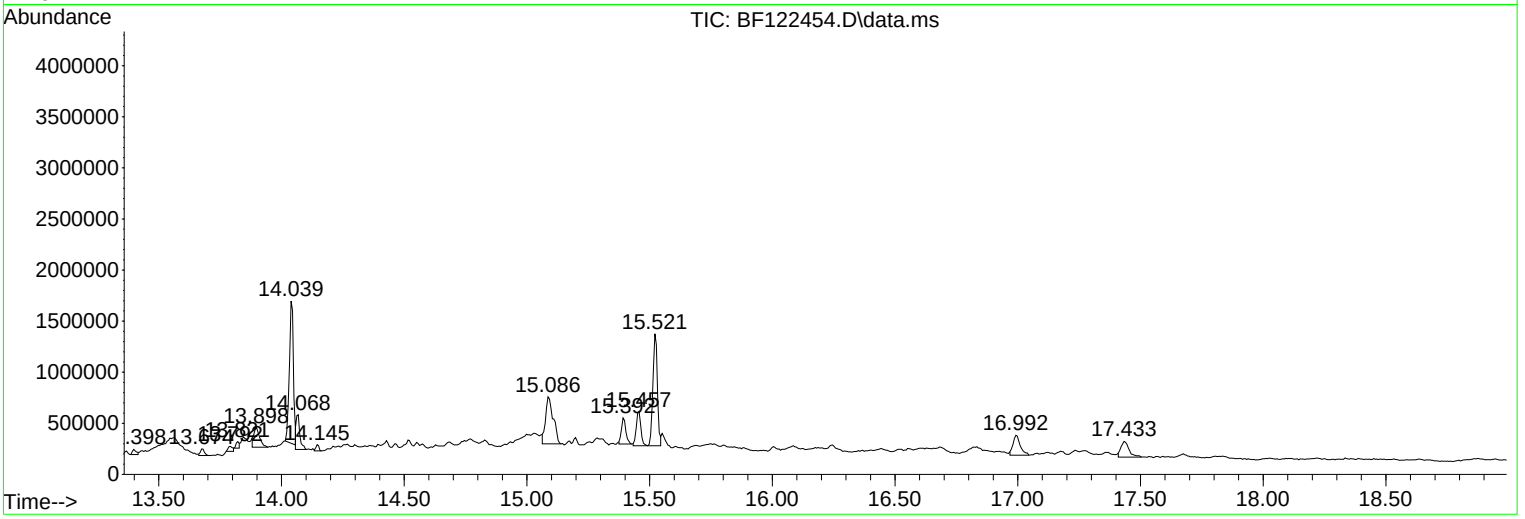
Instrument :
BNA_F
ClientSampleId :
SB-02

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\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02

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

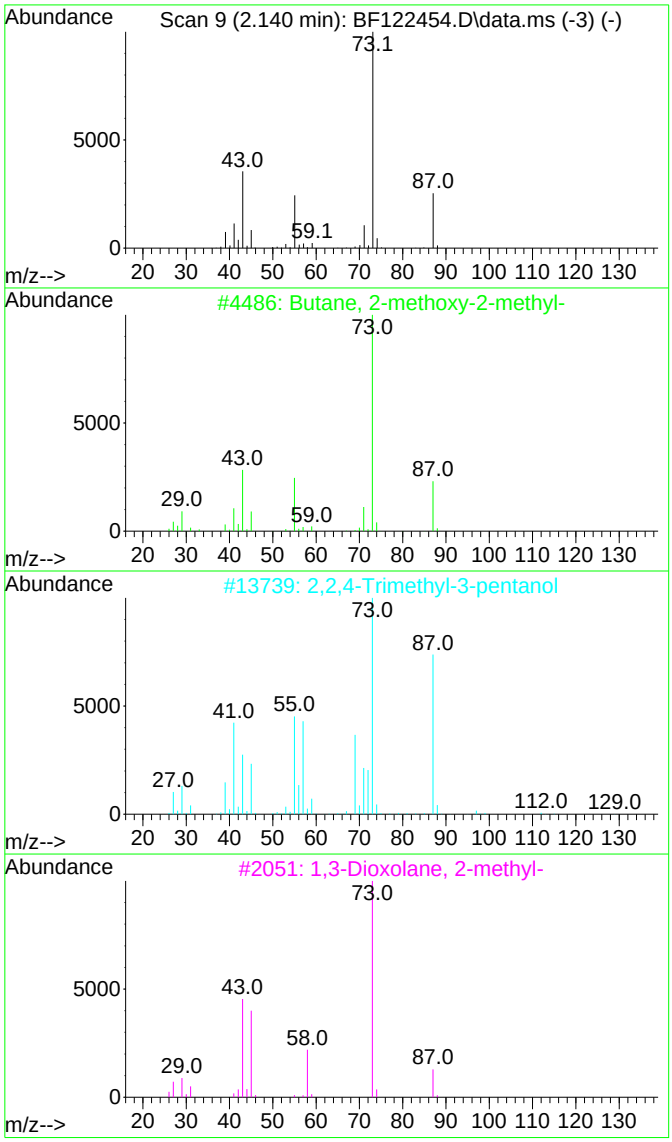
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

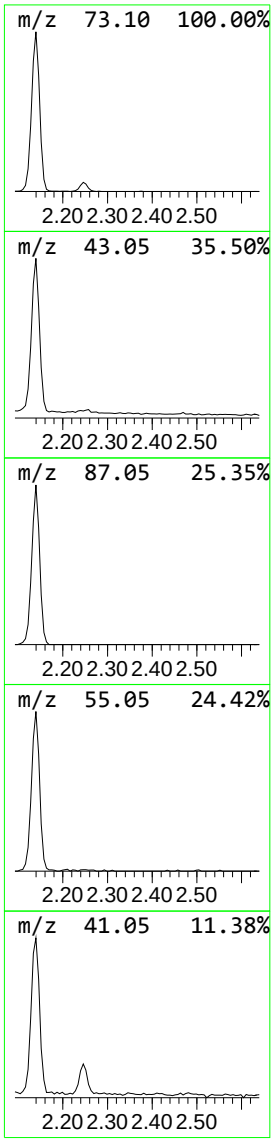
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	12.41 ng	665099	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02

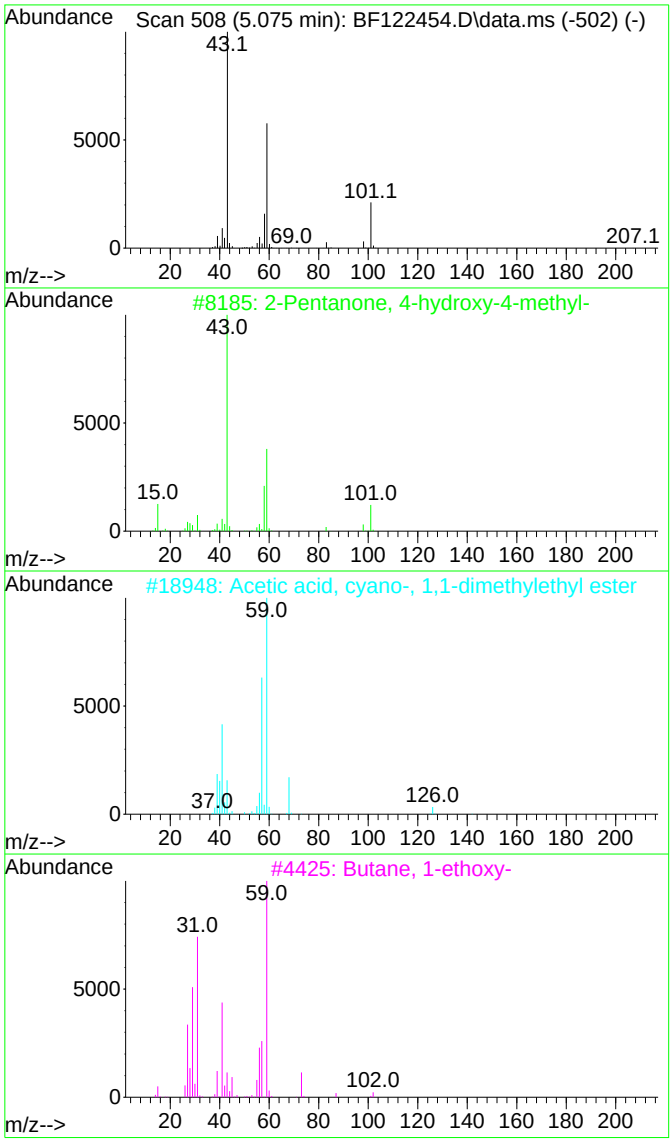
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

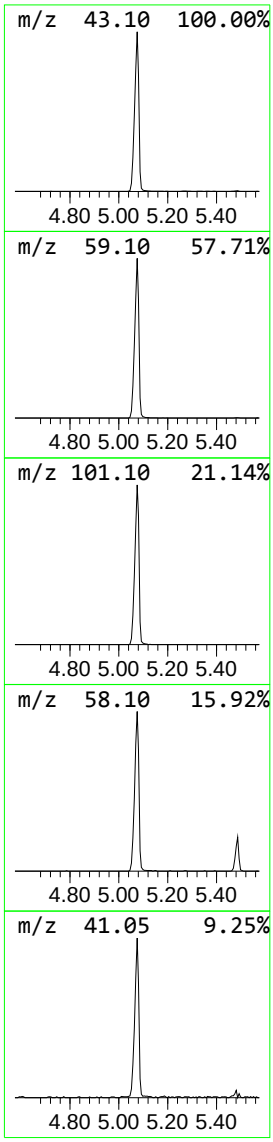
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	36.87 ng	1976540	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02

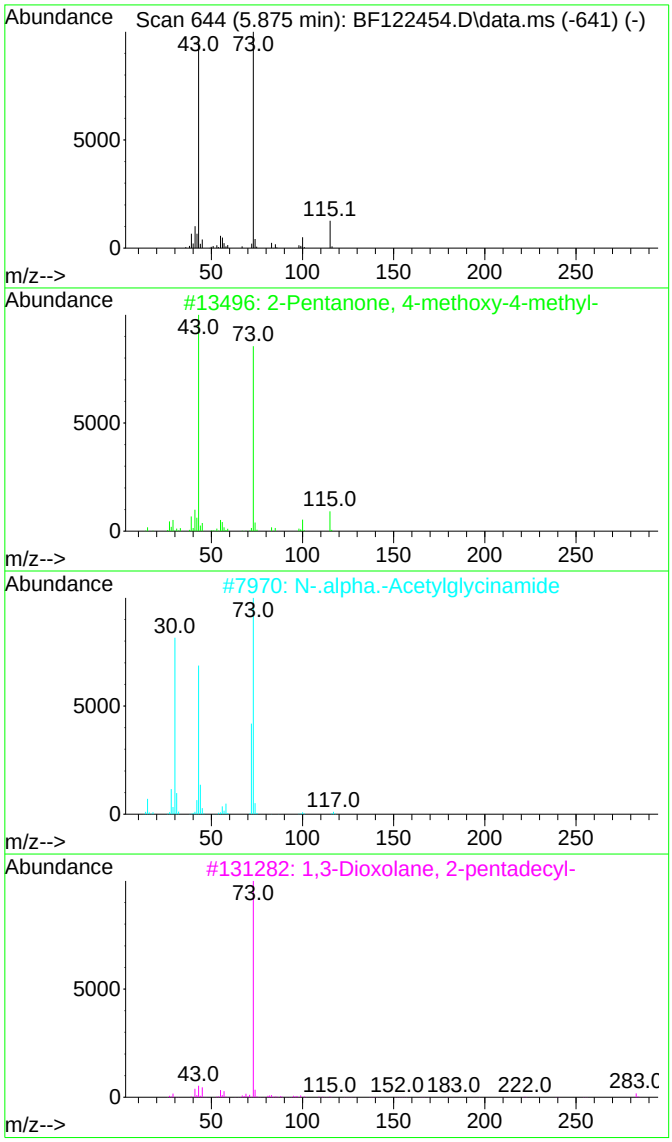
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

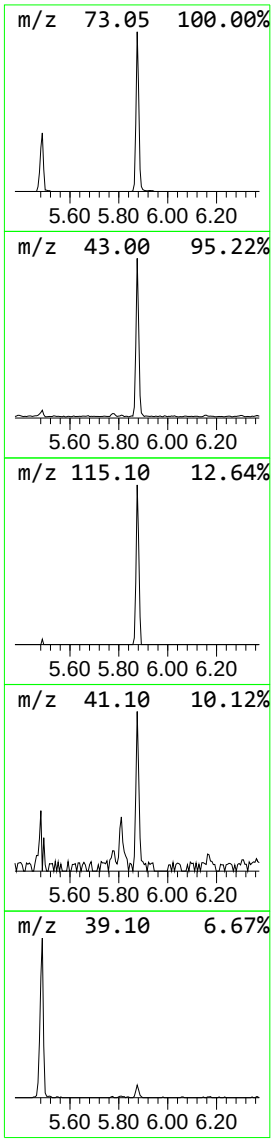
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.875	3.26 ng	174807	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	43
3	1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	17
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02

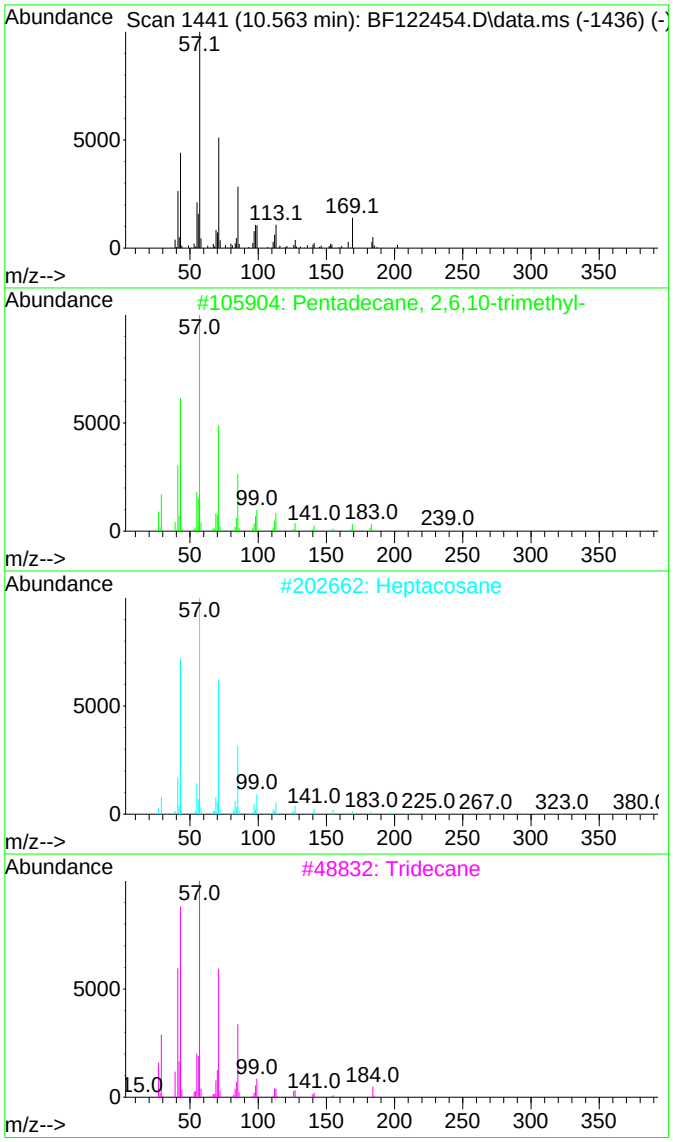
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

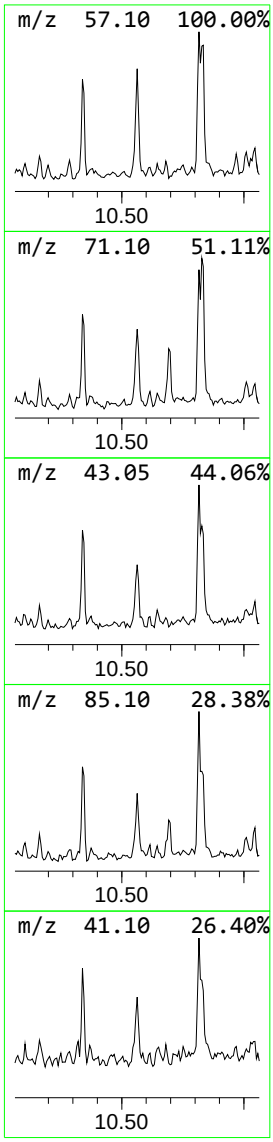
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentadecane, 2,6,10-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.563	2.25 ng	170107	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
2	Heptacosane	380	C27H56	000593-49-7	72
3	Tridecane	184	C13H28	000629-50-5	72
4	Tridecane, 2-methyl-	198	C14H30	001560-96-9	64
5	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02

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

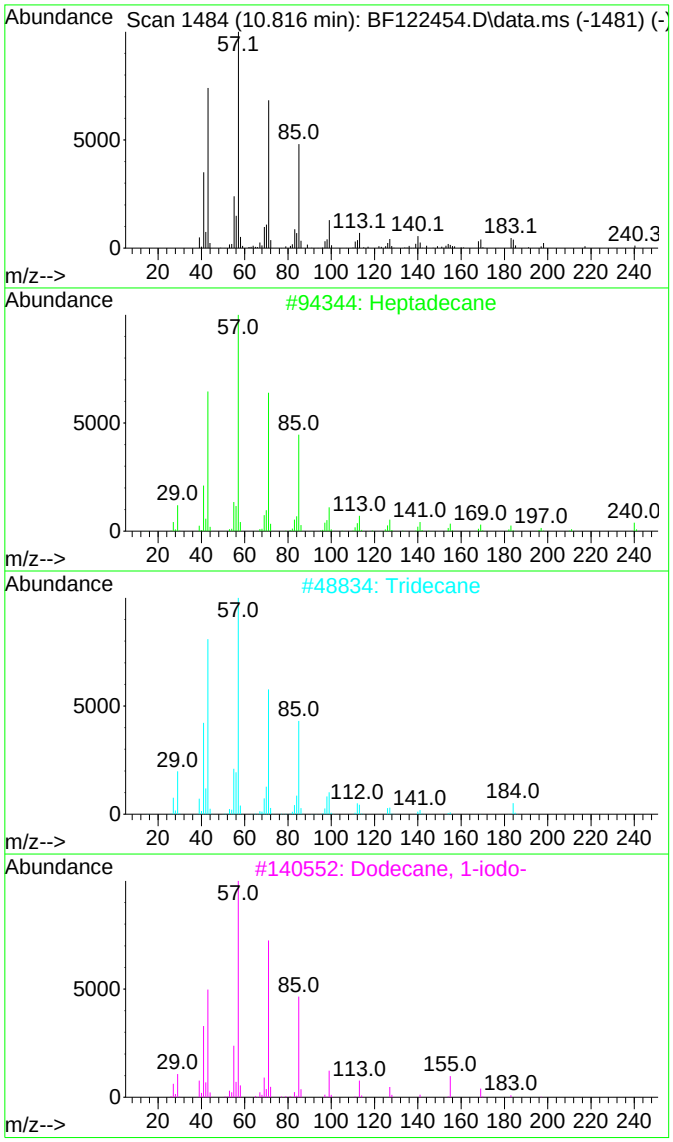
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

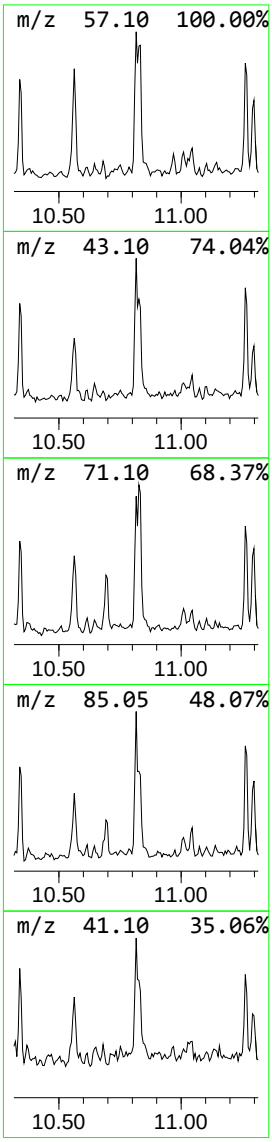
****

Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.816	2.29 ng	153854	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Tridecane	184	C13H28	000629-50-5	91
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80
5	Heneicosane	296	C21H44	000629-94-7	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02

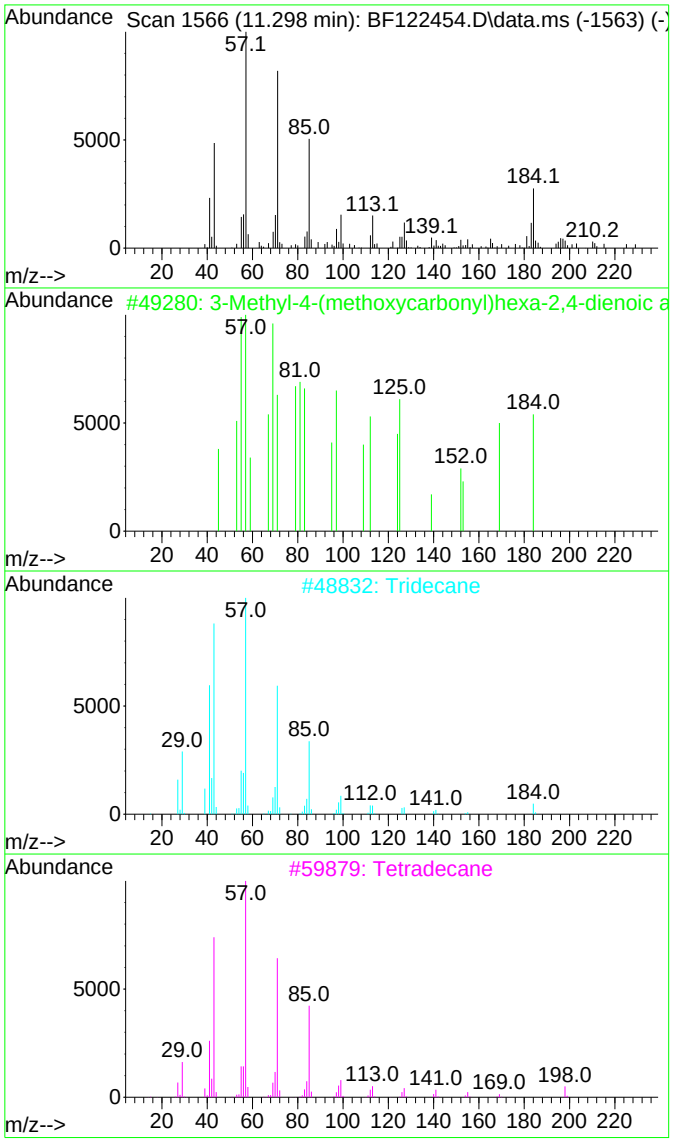
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

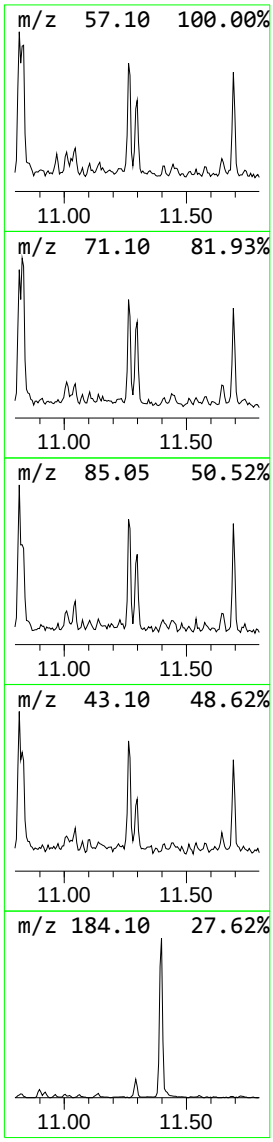
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Methyl-4-(methoxycarbonyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	2.17 ng	146245	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-4-(methoxycarbonyl)hexa...	184	C9H12O4	1000104-10-8	90
2	Tridecane	184	C13H28	000629-50-5	86
3	Tetradecane	198	C14H30	000629-59-4	76
4	Pentadecane	212	C15H32	000629-62-9	74
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02

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

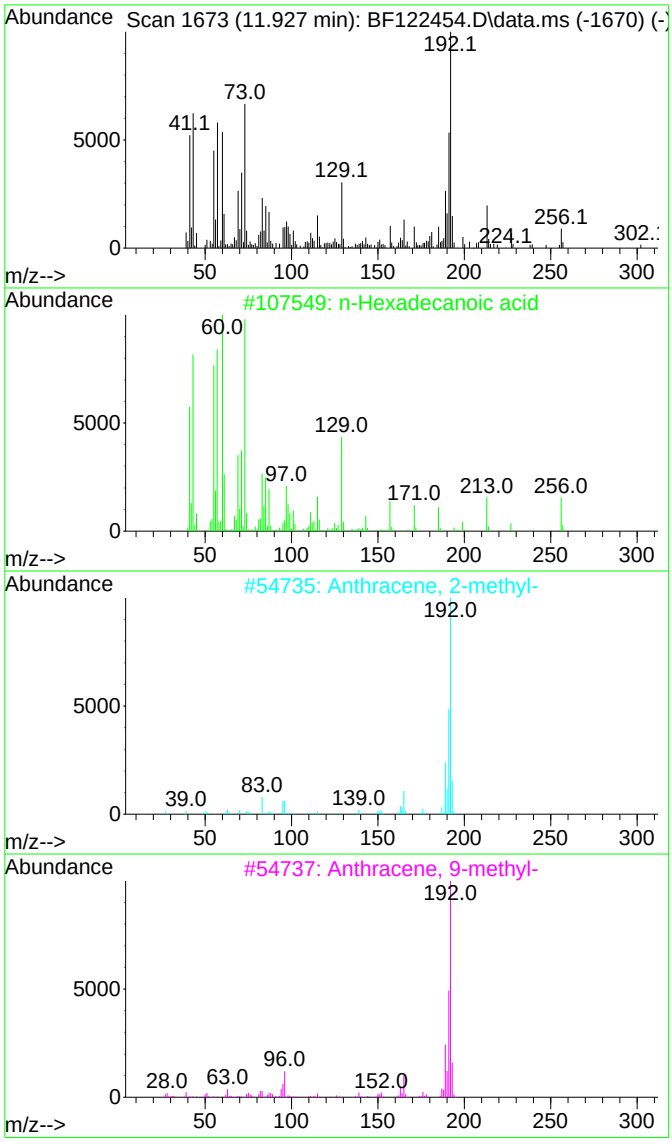
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

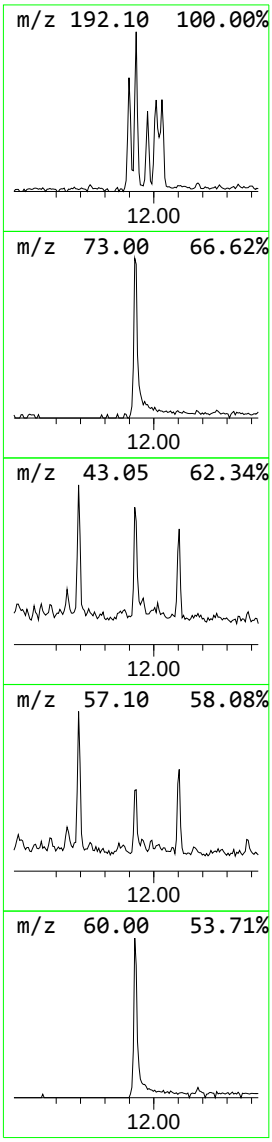
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	3.40 ng	228611	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	64





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Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02

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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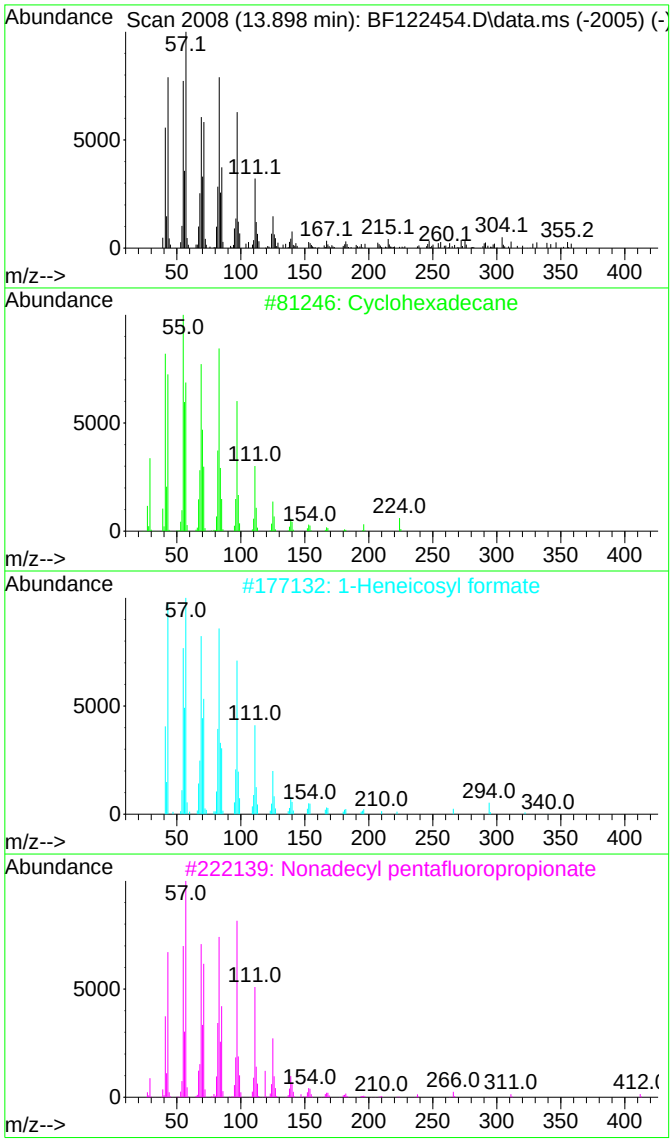
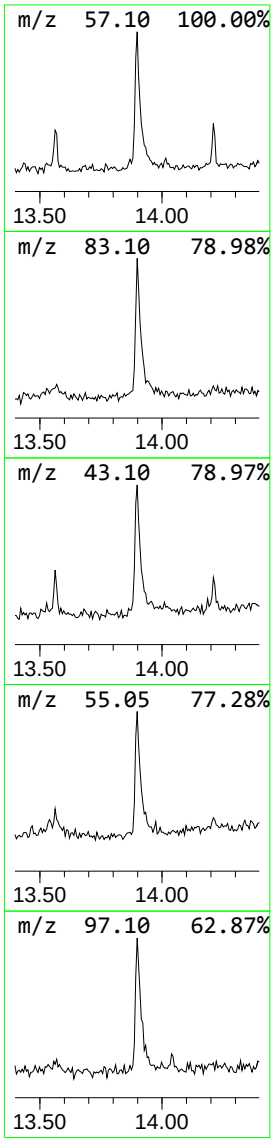
Peak Number 8 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	3.83 ng	308781	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91





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Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02

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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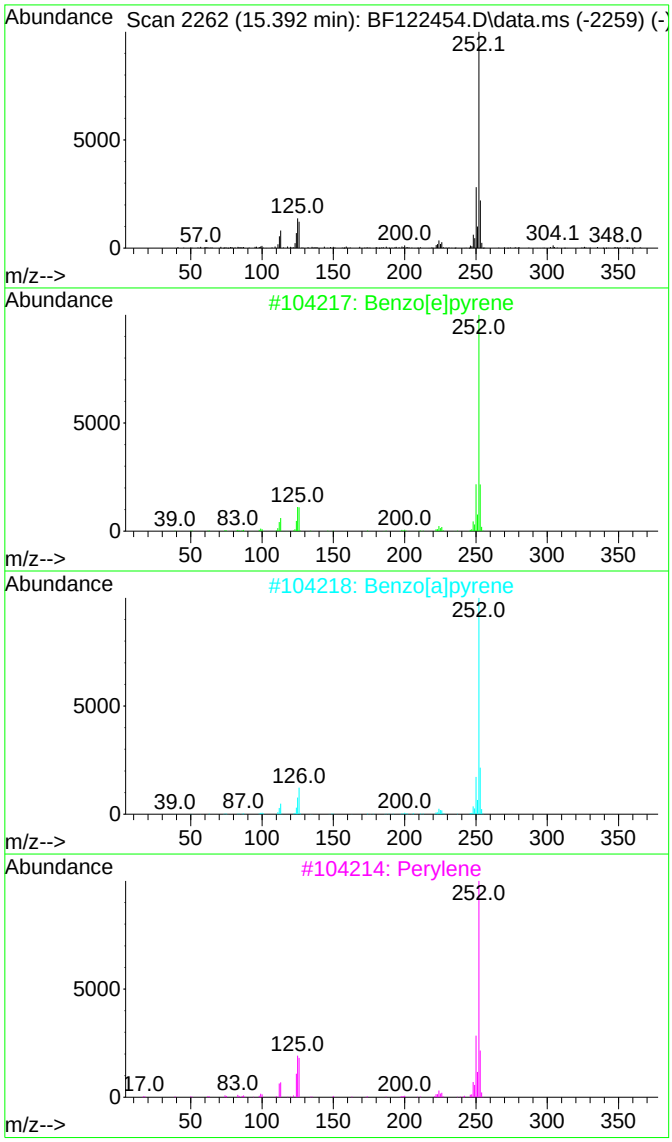
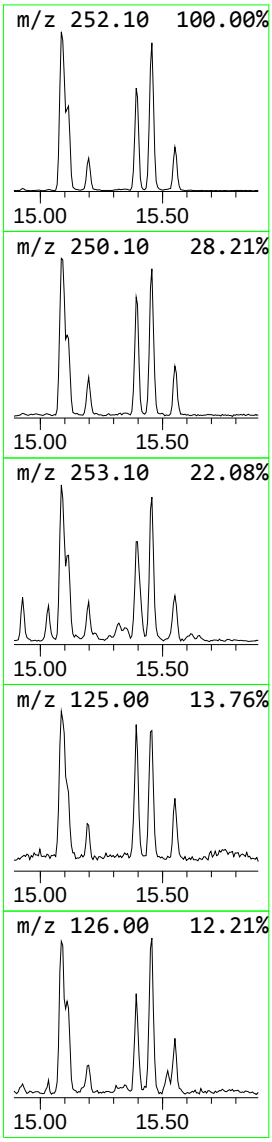
Peak Number 9 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	4.55 ng	320555	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	97
3	Perylene	252	C20H12	000198-55-0	93
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
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Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02

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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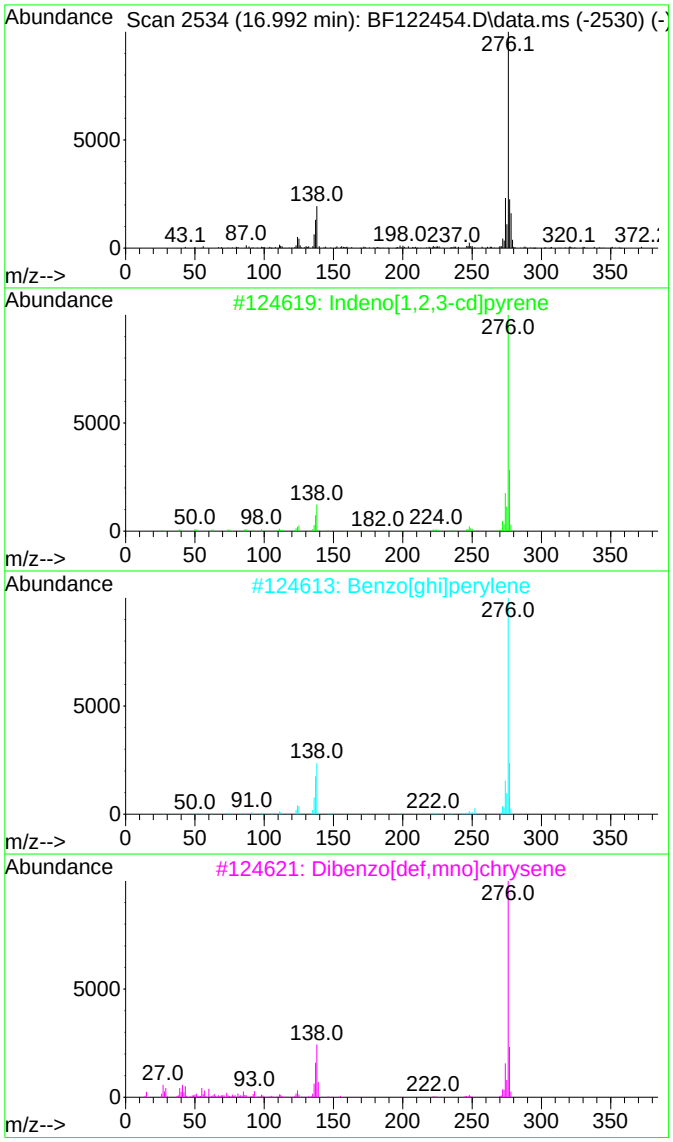
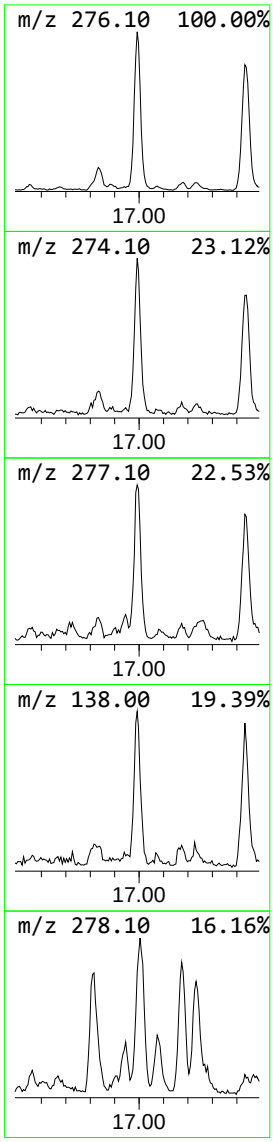
Peak Number 10 Dibenzo[def,mno]chrysene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.992	5.57 ng	392681	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	96
2	Benzo[ghi]perylene	276	C22H12	000191-24-2	93
3	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	81
4	1,2-Propanediol, 1-(1-phenyl-1H-...	320	C18H16N4O2	056804-89-8	47
5	Phosphoric acid, 4-methoxy-2-(me...	276	C11H17O6P	094420-71-0	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122454.D
Acq On : 23 Nov 2020 18:51
Operator : JU/CG
Sample : L4836-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-02

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...	2.140	12.4	ng	665099	1	6.863	1072150	20.0
2-Pentanone, 4-...	5.075	36.9	ng	1976540	1	6.863	1072150	20.0
2-Pentanone, 4-...	5.875	3.3	ng	174807	1	6.863	1072150	20.0
Pentadecane, 2,...	10.563	2.3	ng	170107	3	9.910	1514050	20.0
Heptadecane	10.816	2.3	ng	153854	4	11.398	1345400	20.0
3-Methyl-4-(met...	11.298	2.2	ng	146245	4	11.398	1345400	20.0
n-Hexadecanoic ...	11.927	3.4	ng	228611	4	11.398	1345400	20.0
Cyclohexadecane	13.898	3.8	ng	308781	5	14.045	1611210	20.0
Benzo[e]pyrene	15.392	4.5	ng	320555	6	15.521	1409460	20.0
Dibenzo[def,mno...	16.992	5.6	ng	392681	6	15.521	1409460	20.0