LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124188.D
Acq On : 8 Jun 2021 19:37
Operator : JU/CG
Sample : M2598-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 19

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124188.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	18	rBB	468939	582195	47.66%	6.224%
2	5.081	506	509	514	rVB	20637	23909	1.96%	0.256%
3	5.498	576	580	589	rBV	805885	823846	67.44%	8.808%
4	6.139	687	689	692	rBV	17809	13436	1.10%	0.144%
5	6.504	747	751	764	rBV	801731	844433	69.12%	9.028%
6	6.857	808	811	815	rBV	313830	268253	21.96%	2.868%
7	7.422	902	907	910	rBV	676695	626125	51.25%	6.694%
8	8.139	1025	1029	1033	rBV	355941	335554	27.47%	3.588%
9	9.222	1208	1213	1216	rBV	1377172	1221659	100.00%	13.061%
10	9.898	1324	1328	1331	rBV	515872	401623	32.88%	4.294%
11	10.686	1458	1462	1467	rBV	777329	692010	56.65%	7.399%
12	10.798	1478	1481	1489	rVB2	10267	14212	1.16%	0.152%
13	11.245	1553	1557	1560	rBV2	13556	13438	1.10%	0.144%
14	11.386	1577	1581	1583	rBV	433991	356159	29.15%	3.808%
15	11.410	1583	1585	1588	rVB	115031	82207	6.73%	0.879%
16	11.598	1614	1617	1619	rBV	20382	16719	1.37%	0.179%
17	11.886	1663	1666	1668	rBV2	15470	13534	1.11%	0.145%
18	11.916	1668	1671	1674	rBV3	21602	21222	1.74%	0.227%
19	11.998	1682	1685	1688	rBV4	16908	22194	1.82%	0.237%
20	12.210	1718	1721	1726	rVB6	22634	19812	1.62%	0.212%
21	12.433	1757	1759	1762	rBV3	15078	14020	1.15%	0.150%
22	12.474	1762	1766	1768	rVV4	14789	16006	1.31%	0.171%
23	12.521	1772	1774	1780	rVB5	17185	21693	1.78%	0.232%
24	12.598	1784	1787	1792	rVB	135773	116729	9.55%	1.248%
25	12.645	1792	1795	1800	rBV7	8840	14962	1.22%	0.160%
26	12.827	1821	1826	1831	rBV2	94193	99697	8.16%	1.066%
27	12.974	1846	1851	1854	rBV	1066855	994924	81.44%	10.637%
28	13.074	1866	1868	1871	rVB4	18920	17475	1.43%	0.187%
29	13.204	1887	1890	1892	rBV2	24981	21511	1.76%	0.230%
30	13.851	1998	2000	2002	rBV3	21126	22118	1.81%	0.236%
31	13.874	2002	2004	2009	rVB4	51033	48124	3.94%	0.515%
32	14.027	2024	2030	2033	rBV2	279229	368050	30.13%	3.935%
33	14.057	2033	2035	2039	rVB	62510	53531	4.38%	0.572%
34	14.157	2049	2052	2054	rBV4	42461	42185	3.45%	0.451%
35	14.498	2108	2110	2112	rVB	41199	28503	2.33%	0.305%
36	15.080	2205	2209	2212	rBV2	85436	136246	11.15%	1.457%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
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Acq On : 8 Jun 2021 19:37
Operator : JU/CG
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 19

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.151	2217	2221	2225	rBV	89760	104888	8.59%	1.121%
38	15.386	2259	2261	2265	rVB2	73585	80461	6.59%	0.860%
39	15.451	2269	2272	2274	rBV3	54468	65698	5.38%	0.702%
40	15.515	2279	2283	2290	rVB	204512	297454	24.35%	3.180%
41	16.251	2405	2408	2413	rVB5	84601	126765	10.38%	1.355%
42	16.662	2475	2478	2487	rVB10	42285	94445	7.73%	1.010%
43	16.786	2495	2499	2503	rBV6	37931	53226	4.36%	0.569%
44	17.098	2547	2552	2559	rVB3	45966	93597	7.66%	1.001%
45	18.239	2742	2746	2748	rBV5	20038	28503	2.33%	0.305%

Sum of corrected areas: 9353351

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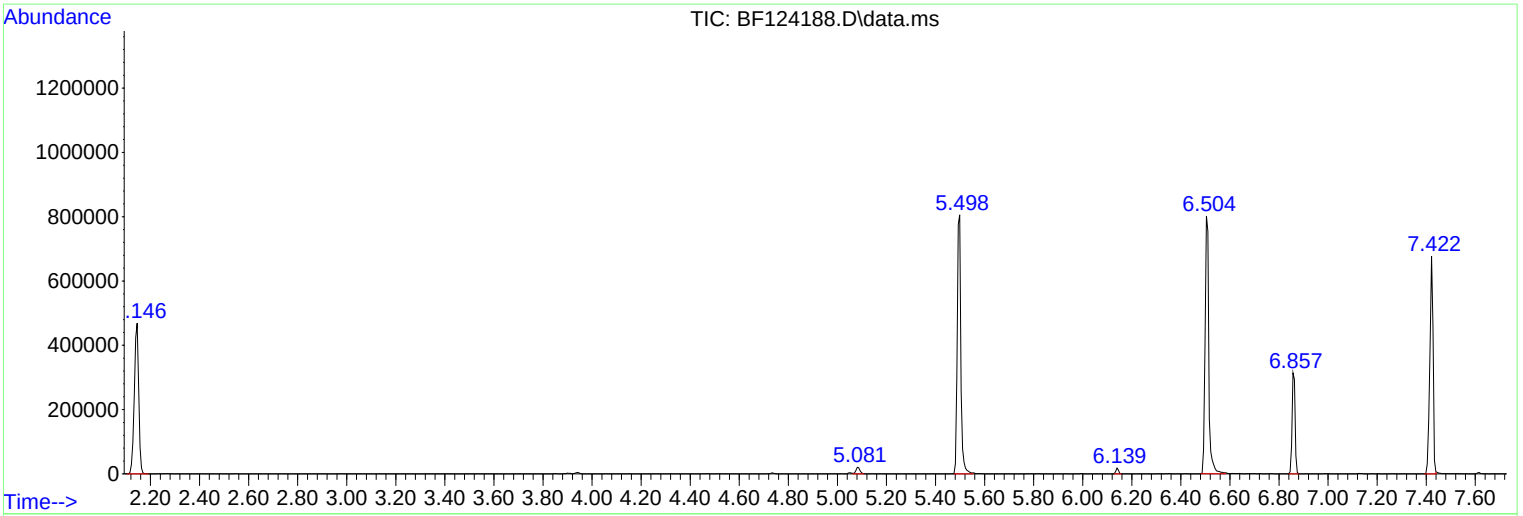
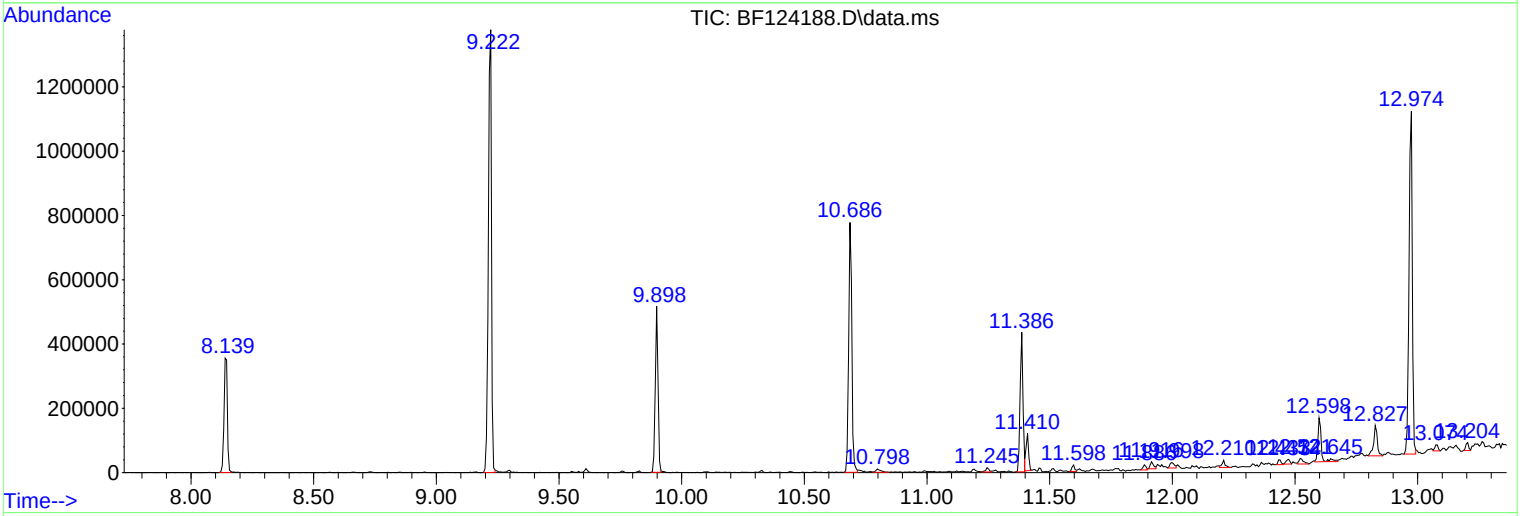
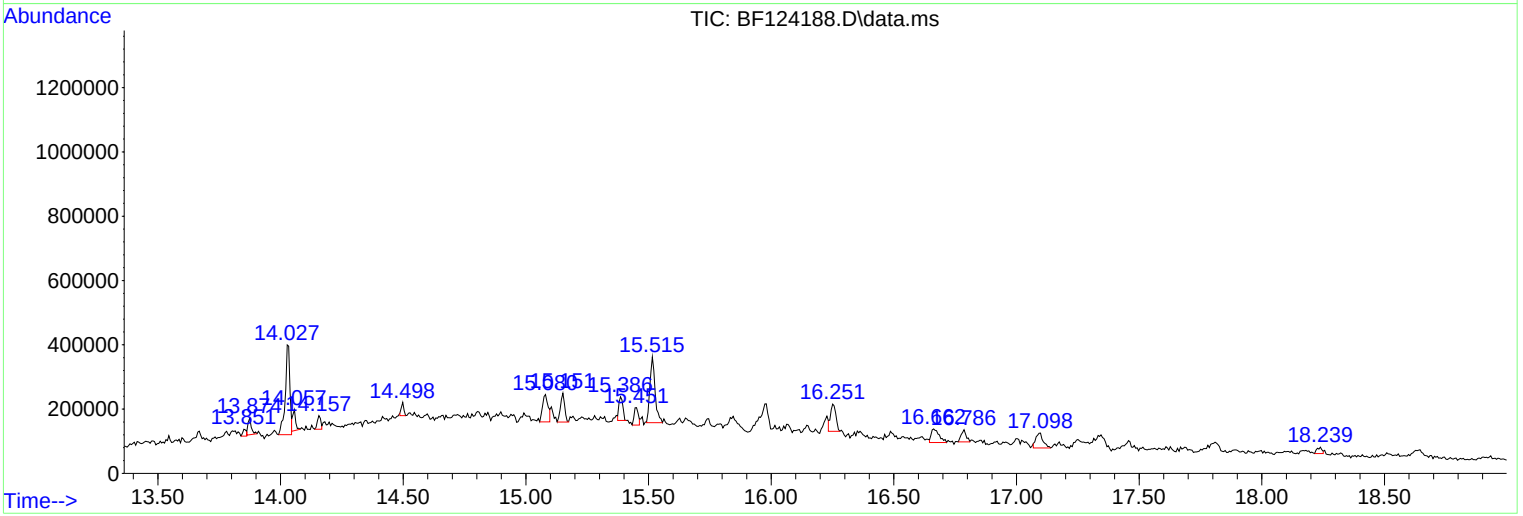
Instrument :
BNA_F
ClientSampleId :
19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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\BF060821\
Data File : BF124188.D
Acq On : 8 Jun 2021 19:37
Operator : JU/CG
Sample : M2598-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
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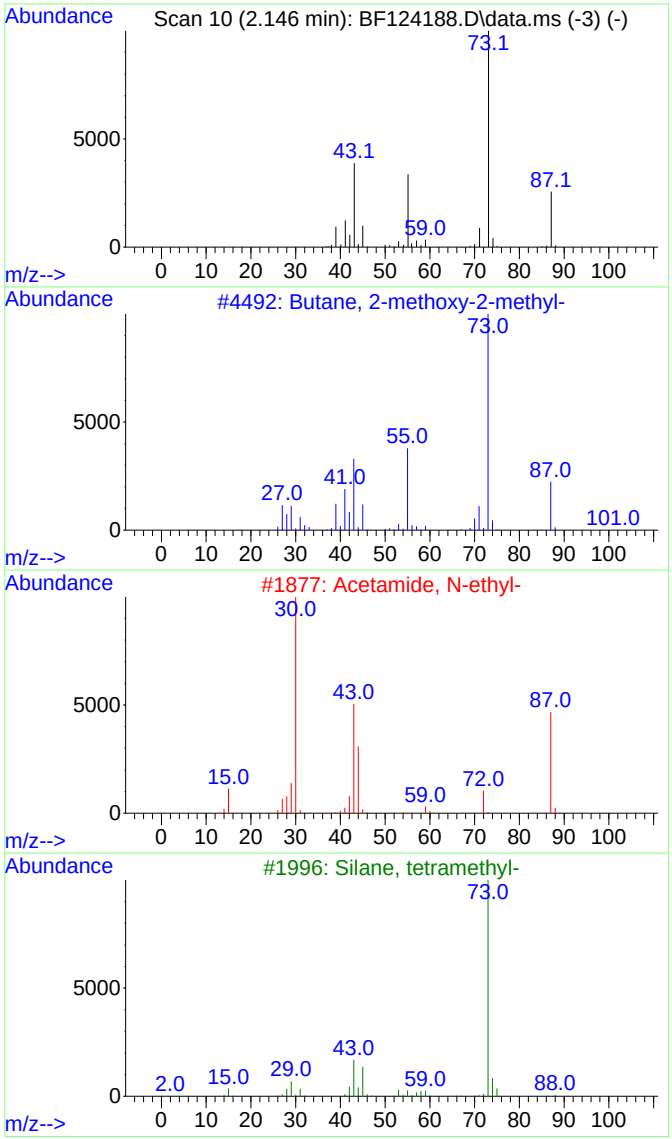
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

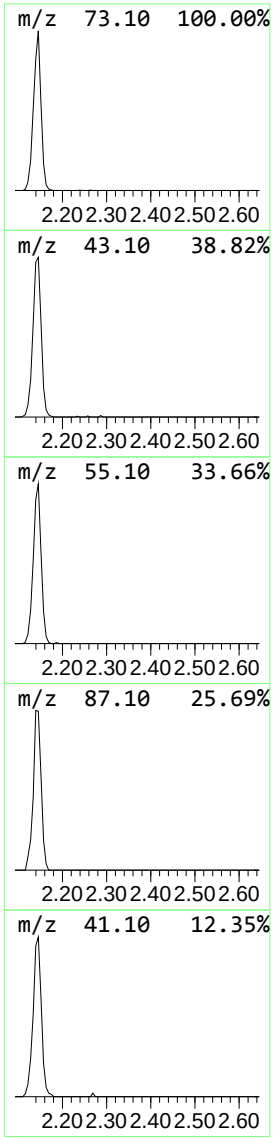
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	43.41 ng	582195	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	72
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	25
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BF124188.D
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Operator : JU/CG
Sample : M2598-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

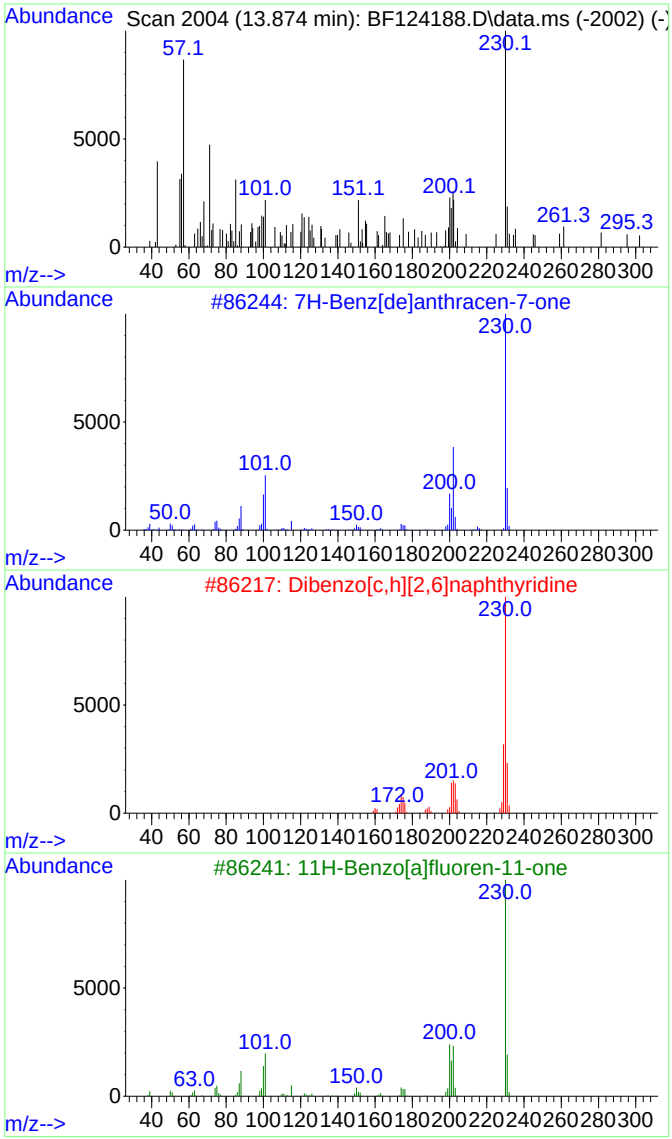
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

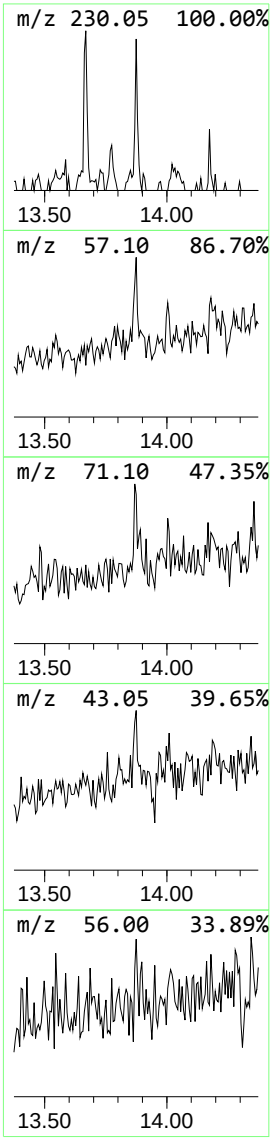
****

Peak Number 2 7H-Benz[de]anthracen-7-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.62 ng	48124	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	55
2	Dibenzo[c,h][2,6]naphthyridine	230	C16H10N2	000218-30-4	47
3	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	46
4	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	42
5	4-(2-(4-Formylphenyl)ethenyl)qui...	259	C18H13NO	082964-46-3	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124188.D
Acq On : 8 Jun 2021 19:37
Operator : JU/CG
Sample : M2598-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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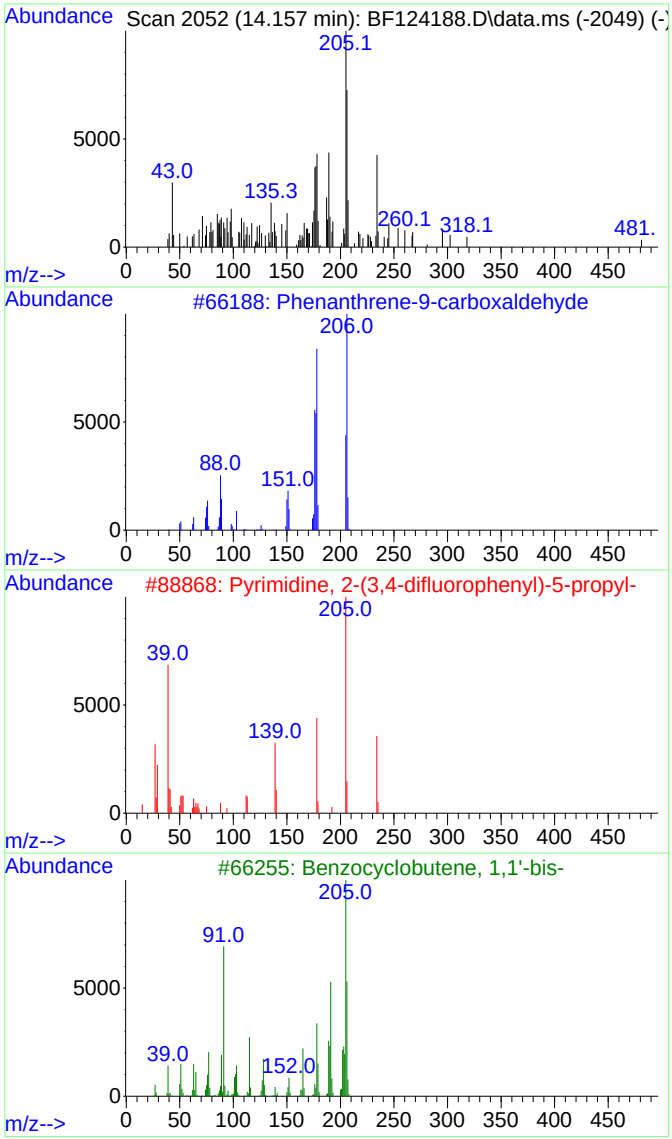
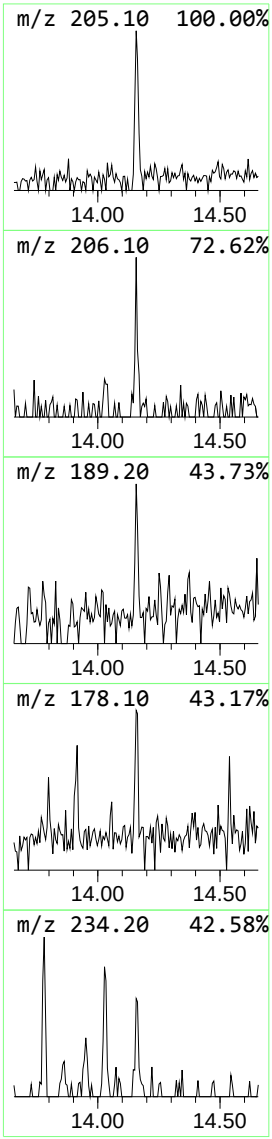
Peak Number 3 unknown14.156 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.156	2.29 ng	42185	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene-9-carboxaldehyde	206	C15H10O	004707-71-5	42
2	Pyrimidine, 2-(3,4-difluoropheny...	234	C13H12F2N2	107392-35-8	38
3	Benzocyclobutene, 1,1'-bis-	206	C16H14	121754-51-6	35
4	4H-1-Benzopyran-6-carboxaldehyde...	234	C12H10O5	007338-51-4	27
5	Benzothieno[2,3-d]pyrimidin-4(3H...	206	C10H10N2OS	014346-24-8	14





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Data File : BF124188.D
Acq On : 8 Jun 2021 19:37
Operator : JU/CG
Sample : M2598-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

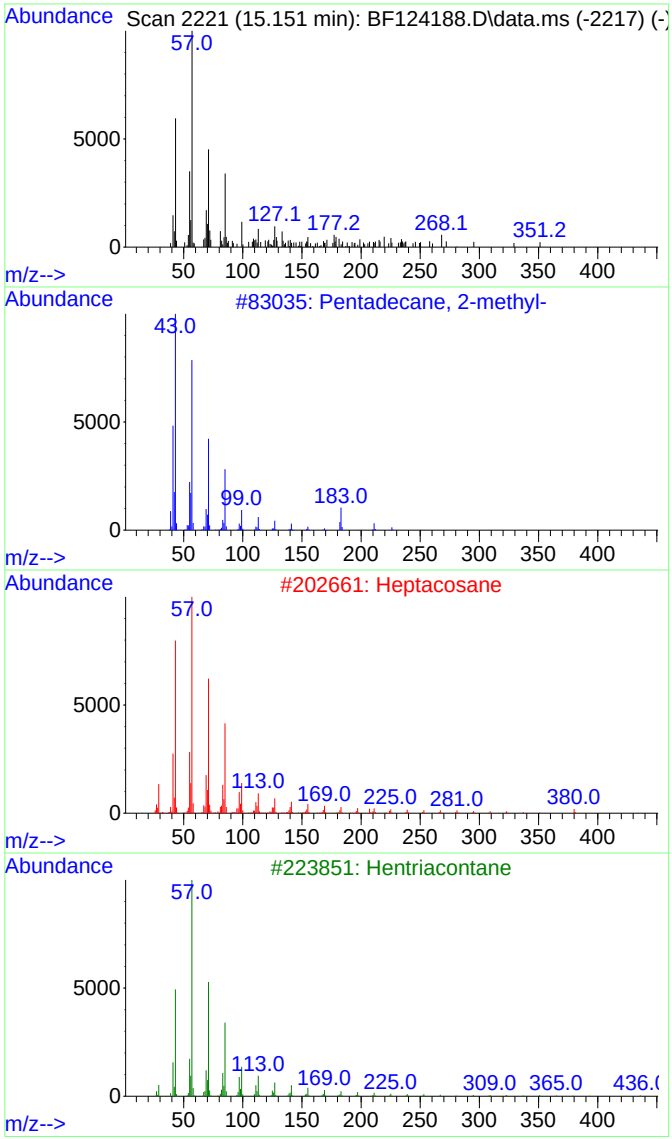
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

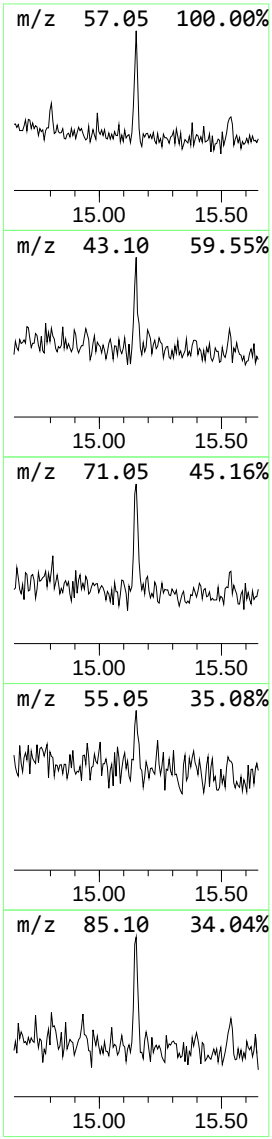
****

Peak Number 4 Pentadecane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	7.05 ng	104888	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	87
2	Heptacosane	380	C27H56	000593-49-7	80
3	Hentriacontane	437	C31H64	000630-04-6	80
4	Pentadecane	212	C15H32	000629-62-9	76
5	Tridecane	184	C13H28	000629-50-5	76





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Instrument : BNA_F
ClientSampleId : 19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

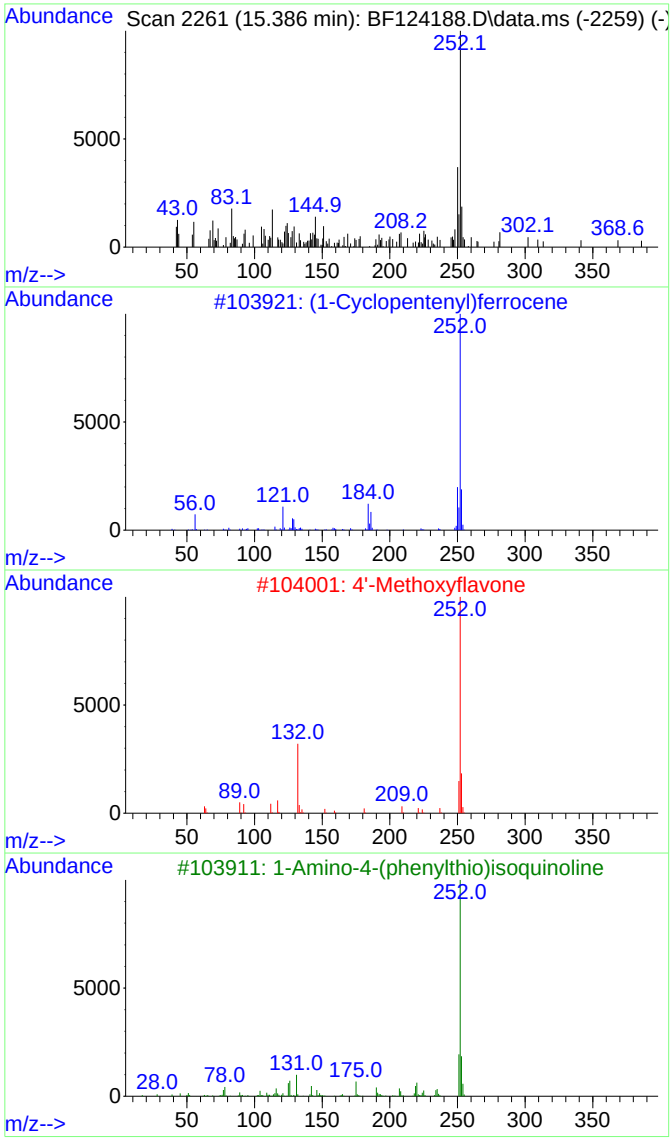
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

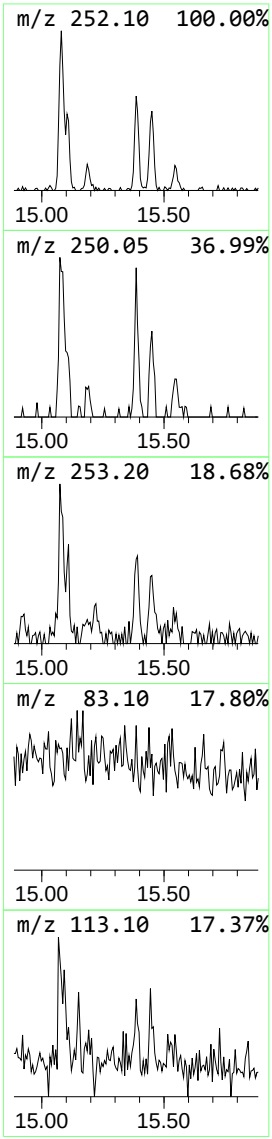
****

Peak Number 5 (1-Cyclopentenyl)ferrocene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	5.41 ng	80461	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	72
2	4'-Methoxyflavone	252	C16H12O3	004143-74-2	70
3	1-Amino-4-(phenylthio)isoquinoline	252	C15H12N2S	019653-19-1	62
4	2-Pyridinamine, 3,5-dibromo-	250	C5H4Br2N2	035486-42-1	58
5	Benzo[b]naphtho[2,3-d]thiophene,...	252	C17H16S	024964-04-3	53





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Instrument : BNA_F
ClientSampleId : 19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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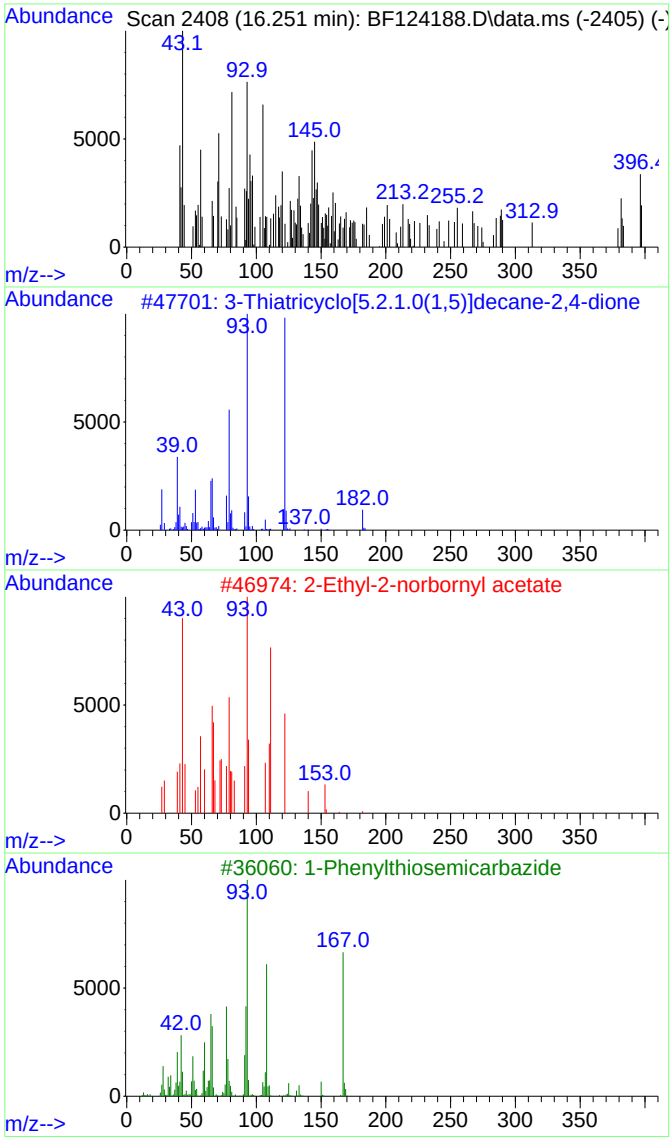
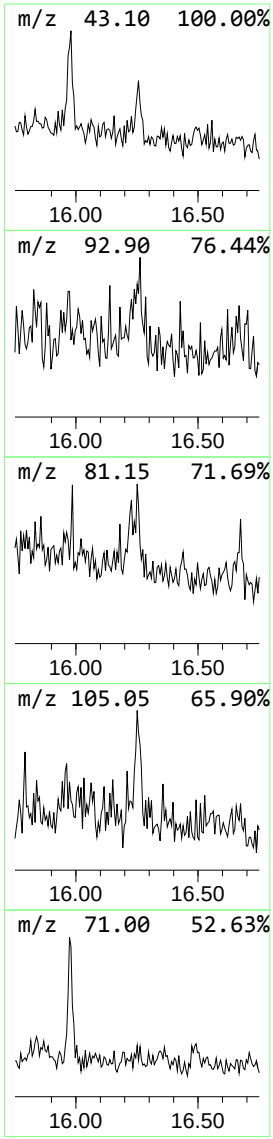
Peak Number 6 unknown16.250 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.250	8.52 ng	126765	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Thiatricyclo[5.2.1.0(1,5)]deca...	182	C9H10O2S	1000187-21-7	35
2	2-Ethyl-2-norbornyl acetate	182	C11H18O2	052352-83-7	25
3	1-Phenylthiosemicarbazide	167	C7H9N3S	000645-48-7	25
4	6-[Phenylcarbamoyl]-2,4-diamino-...	270	C13H14N6O	1000227-45-6	25
5	2-Pyridineacetic acid	137	C7H7NO2	013115-43-0	25





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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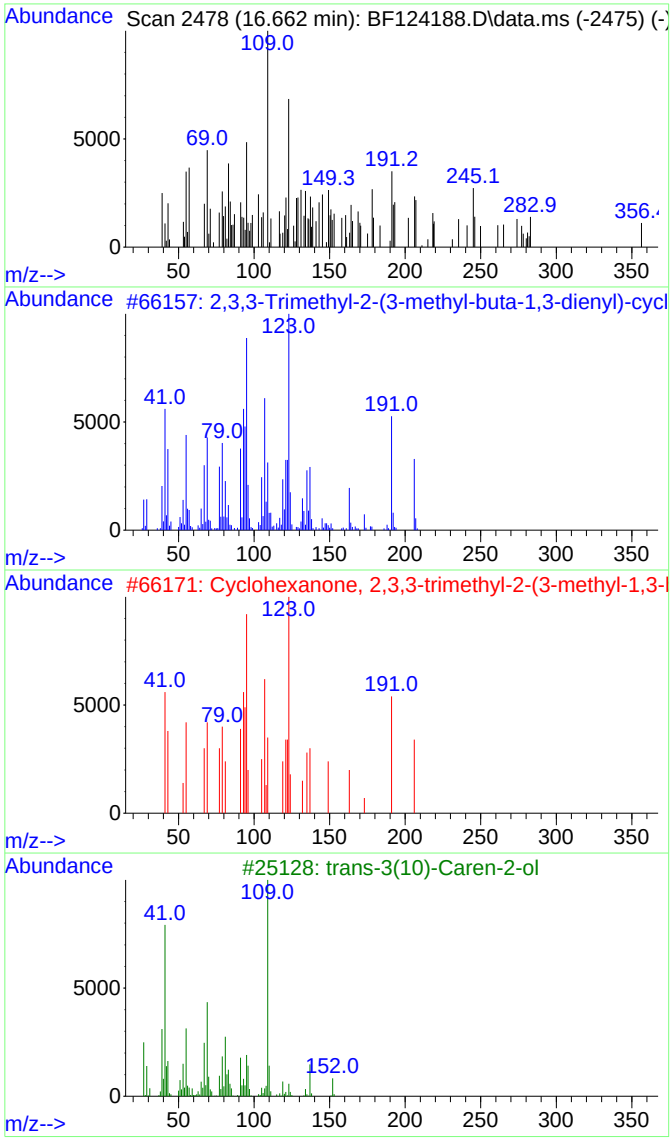
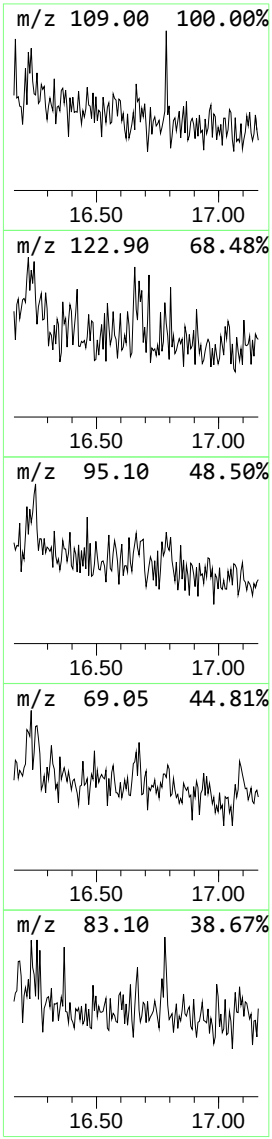
Peak Number 7 unknown16.662 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.662	6.35 ng	94445	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	30
2	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	30
3	trans-3(10)-Caren-2-ol	152	C10H16O	1000151-66-5	25
4	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	22
5	N-(4-Methyl-2-pyrimidinyl)acetoa...	193	C9H11N3O2	000713-70-2	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124188.D
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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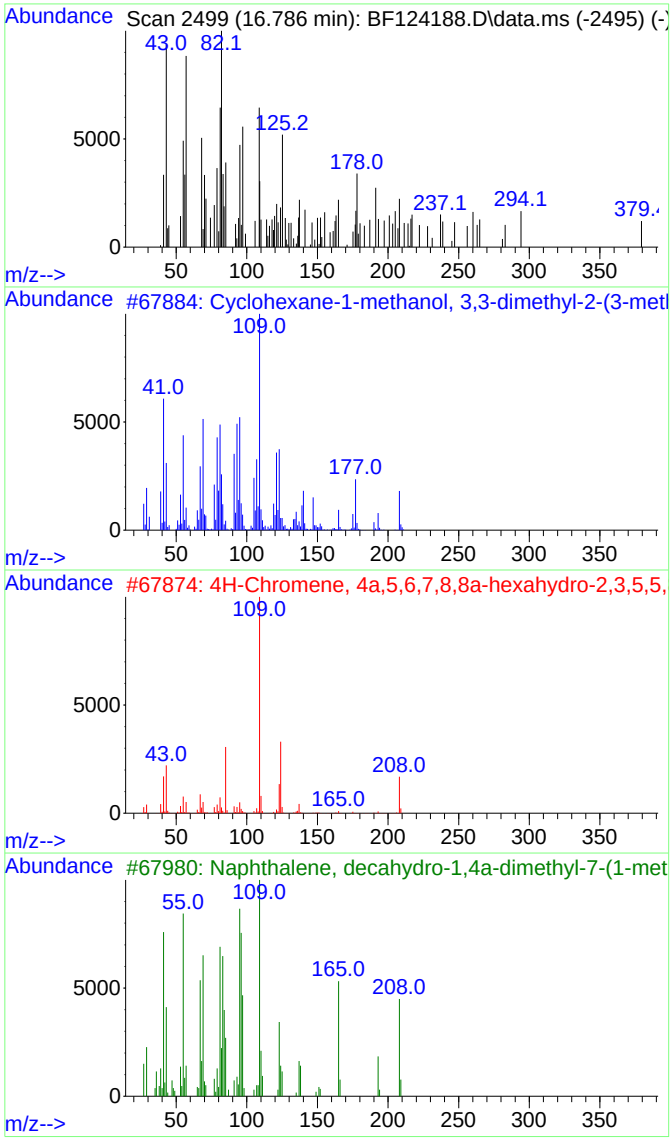
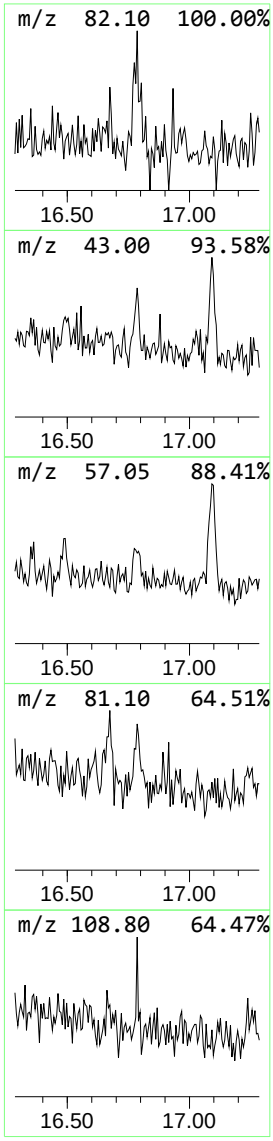
Peak Number 8 unknown16.786 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.786	3.58 ng	53226	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane-1-methanol, 3,3-dime...	208	C14H24O	1000196-01-5	38
2	4H-Chromene, 4a,5,6,7,8,8a-hexah...	208	C14H24O	1000196-77-4	30
3	Naphthalene, decahydro-1,4a-dime...	208	C15H28	030824-81-8	25
4	N-(1-Cyano-3-methyl-but-2-enyl)-...	152	C8H12N2O	1000192-62-7	22
5	p-Nitrophenyl nonyl ether	265	C15H23NO3	086702-46-7	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124188.D
Acq On : 8 Jun 2021 19:37
Operator : JU/CG
Sample : M2598-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

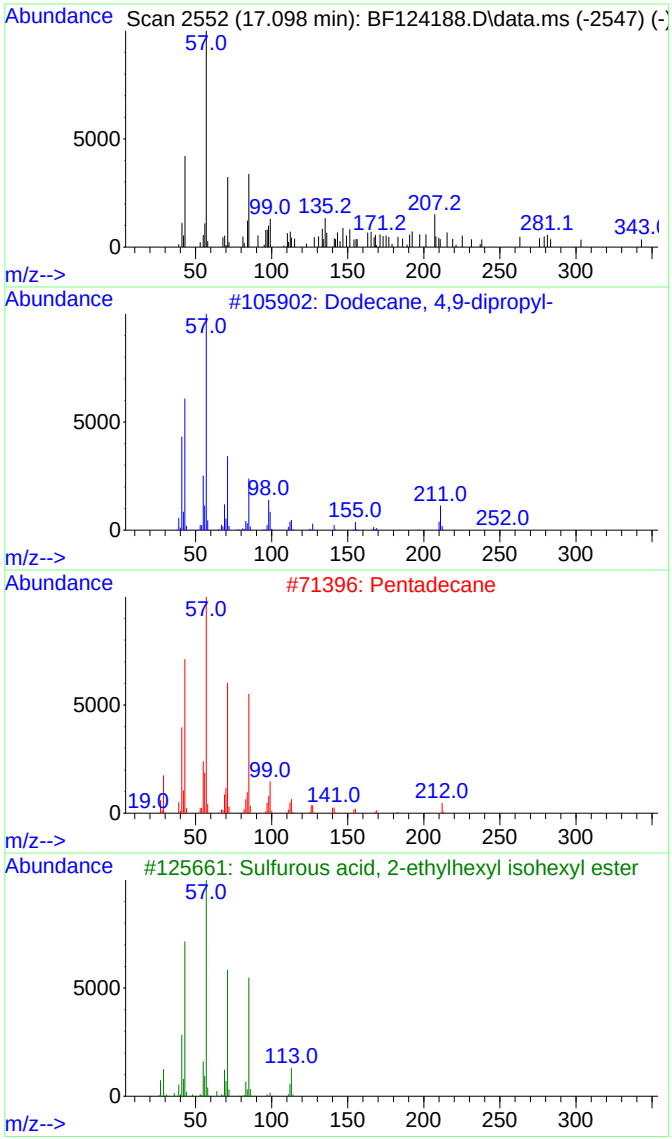
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

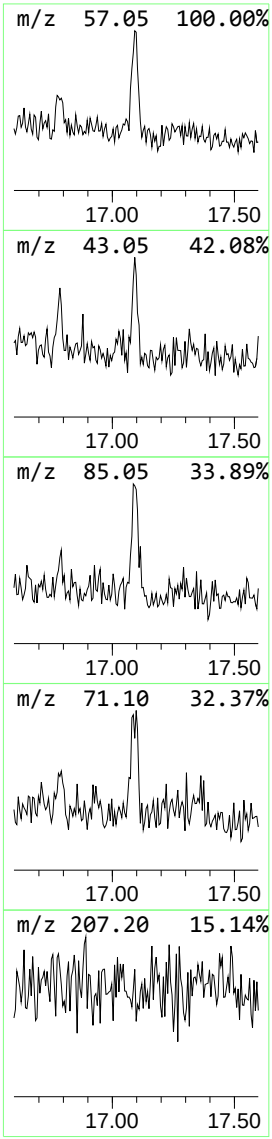
****

Peak Number 9 unknown17.098 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.098	6.29 ng	93597	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 4,9-dipropyl-	254	C18H38	003054-63-5	22
2	Pentadecane	212	C15H32	000629-62-9	14
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	14
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	14
5	Undecane	156	C11H24	001120-21-4	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124188.D
Acq On : 8 Jun 2021 19:37
Operator : JU/CG
Sample : M2598-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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...	2.146	43.4	ng	582195	1	6.863	268253	20.0
7H-Benz[de]anth...	13.874	2.6	ng	48124	5	14.033	368050	20.0
unknown14.156	14.156	2.3	ng	42185	5	14.033	368050	20.0
Pentadecane, 2-...	15.151	7.0	ng	104888	6	15.515	297454	20.0
(1-Cyclopenteny...	15.386	5.4	ng	80461	6	15.515	297454	20.0
unknown16.250	16.250	8.5	ng	126765	6	15.515	297454	20.0
unknown16.662	16.662	6.3	ng	94445	6	15.515	297454	20.0
unknown16.786	16.786	3.6	ng	53226	6	15.515	297454	20.0
unknown17.098	17.098	6.3	ng	93597	6	15.515	297454	20.0