LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123972.D
Acq On : 17 May 2021 19:54
Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123972.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	5	13	19	rVB	476256	617207	56.29%	6.472%
2	2.269	26	31	38	rVB	35885	44842	4.09%	0.470%
3	5.122	513	516	519	rVB2	12693	13846	1.26%	0.145%
4	5.516	578	583	586	rBV	1119980	987964	90.11%	10.360%
5	6.522	749	754	757	rBV	1109701	988505	90.16%	10.366%
6	6.722	786	788	795	rBV	30124	25724	2.35%	0.270%
7	6.904	815	819	822	rBV	335999	257557	23.49%	2.701%
8	7.463	909	914	917	rBV	811000	645916	58.91%	6.773%
9	8.186	1033	1037	1040	rBV	414667	318453	29.04%	3.339%
10	9.263	1216	1220	1223	rBV	1451569	1096450	100.00%	11.498%
11	9.651	1283	1286	1292	rVB	137108	102326	9.33%	1.073%
12	9.939	1332	1335	1339	rVB	425532	343616	31.34%	3.603%
13	10.727	1465	1469	1472	rBV	835222	674039	61.47%	7.068%
14	11.427	1584	1588	1591	rBV	421425	352990	32.19%	3.702%
15	11.451	1591	1592	1595	rVB	60328	33449	3.05%	0.351%
16	11.951	1674	1677	1684	rVB2	96622	83509	7.62%	0.876%
17	12.039	1689	1692	1695	rBV3	16607	17100	1.56%	0.179%
18	12.480	1764	1767	1769	rBV3	12330	14408	1.31%	0.151%
19	12.639	1791	1794	1797	rBV	127610	113664	10.37%	1.192%
20	12.739	1808	1811	1815	rBV4	16251	22060	2.01%	0.231%
21	12.868	1827	1833	1839	rBV	121936	142248	12.97%	1.492%
22	13.015	1854	1858	1861	rBV	1250303	1014449	92.52%	10.638%
23	13.086	1867	1870	1877	rBV9	14290	26781	2.44%	0.281%
24	13.174	1883	1885	1888	rBV4	13640	16952	1.55%	0.178%
25	13.198	1888	1889	1892	rVB3	32713	23597	2.15%	0.247%
26	13.262	1898	1900	1902	rVB2	19524	14226	1.30%	0.149%
27	13.304	1904	1907	1910	rVB3	16633	20330	1.85%	0.213%
28	13.398	1919	1923	1925	rVB5	21945	23118	2.11%	0.242%
29	13.427	1925	1928	1931	rBV5	14608	24531	2.24%	0.257%
30	13.851	1997	2000	2001	rBV3	16248	15860	1.45%	0.166%
31	13.868	2001	2003	2005	rBV3	16044	13903	1.27%	0.146%
32	13.915	2008	2011	2016	rVV	161719	174105	15.88%	1.826%
33	14.068	2032	2037	2040	rBV2	377625	414351	37.79%	4.345%
34	14.092	2040	2041	2044	rVB	57644	43180	3.94%	0.453%
35	14.551	2117	2119	2122	rVB4	32191	24922	2.27%	0.261%
36	14.939	2183	2185	2188	rVB4	35648	25909	2.36%	0.272%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123972.D
Acq On : 17 May 2021 19:54
Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.127	2214	2217	2220	rBV2	63104	77546	7.07%	0.813%
38	15.433	2265	2269	2272	rBV4	57289	90287	8.23%	0.947%
39	15.498	2277	2280	2282	rBV2	42305	41772	3.81%	0.438%
40	15.568	2287	2292	2295	rBV	168279	214879	19.60%	2.253%
41	15.733	2316	2320	2326	rVB8	41777	68049	6.21%	0.714%
42	16.309	2414	2418	2430	rVB8	70293	138520	12.63%	1.453%
43	16.550	2457	2459	2460	rBV2	22763	16422	1.50%	0.172%
44	17.356	2593	2596	2604	rVB10	32982	55942	5.10%	0.587%
45	17.427	2606	2608	2610	rBV3	15998	17304	1.58%	0.181%
46	17.739	2657	2661	2662	rBV4	10632	14340	1.31%	0.150%
47	18.409	2773	2775	2778	rBV4	9416	14764	1.35%	0.155%
48	18.639	2811	2814	2815	rBV3	10406	14293	1.30%	0.150%

Sum of corrected areas: 9536205

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
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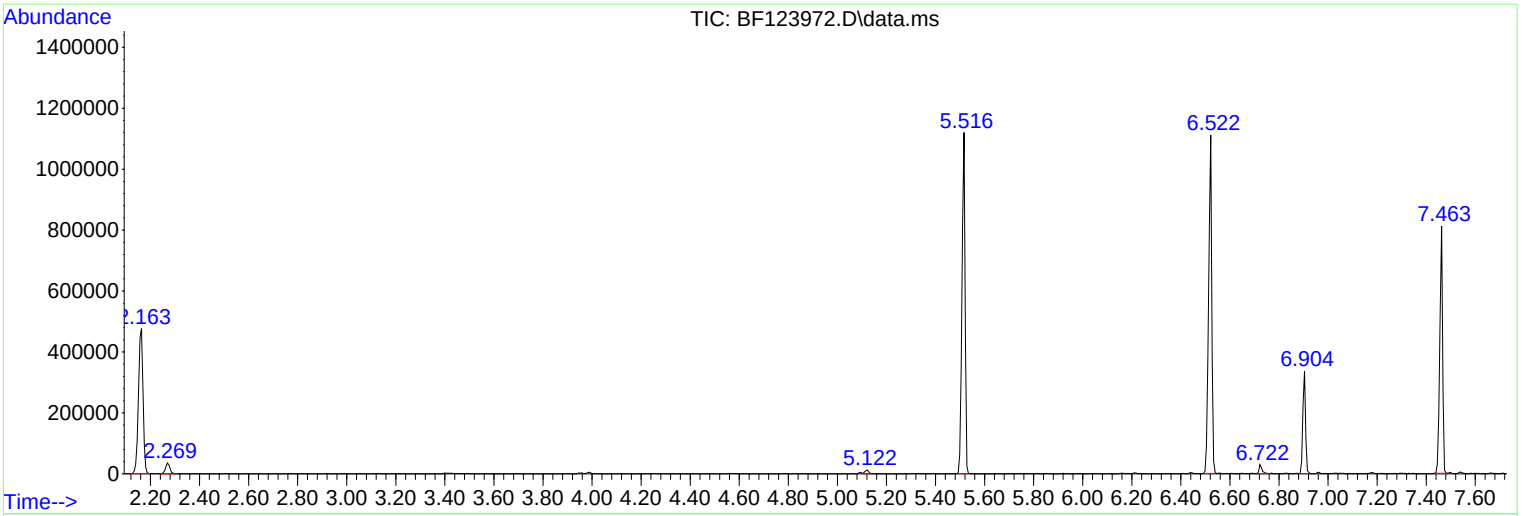
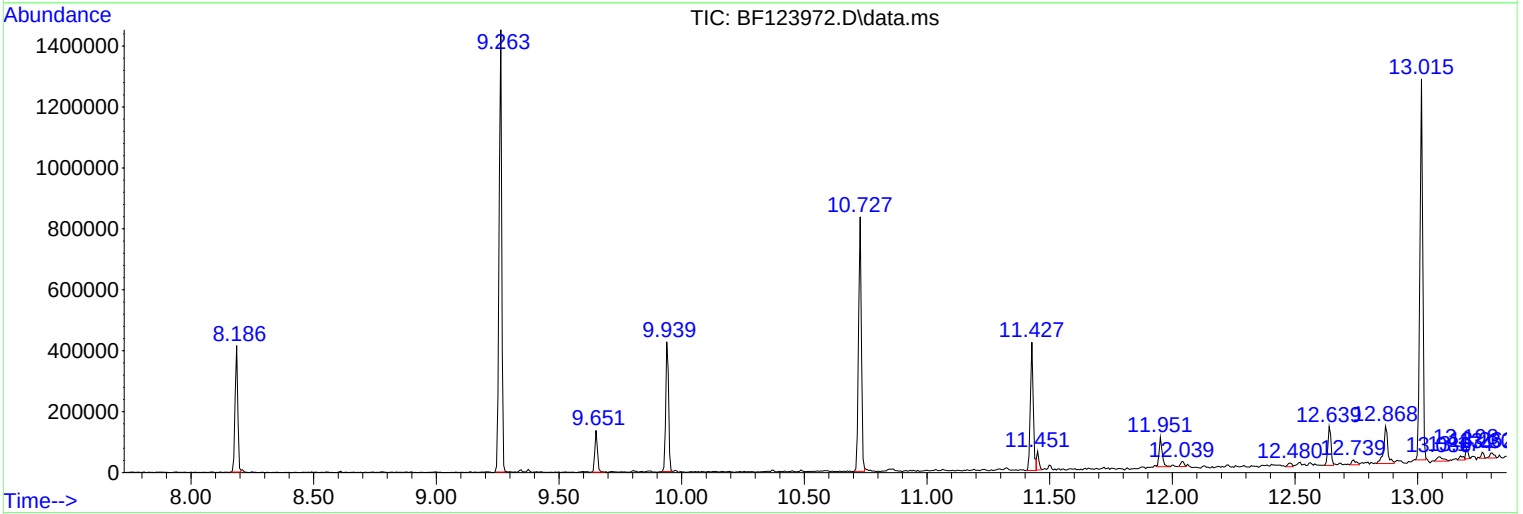
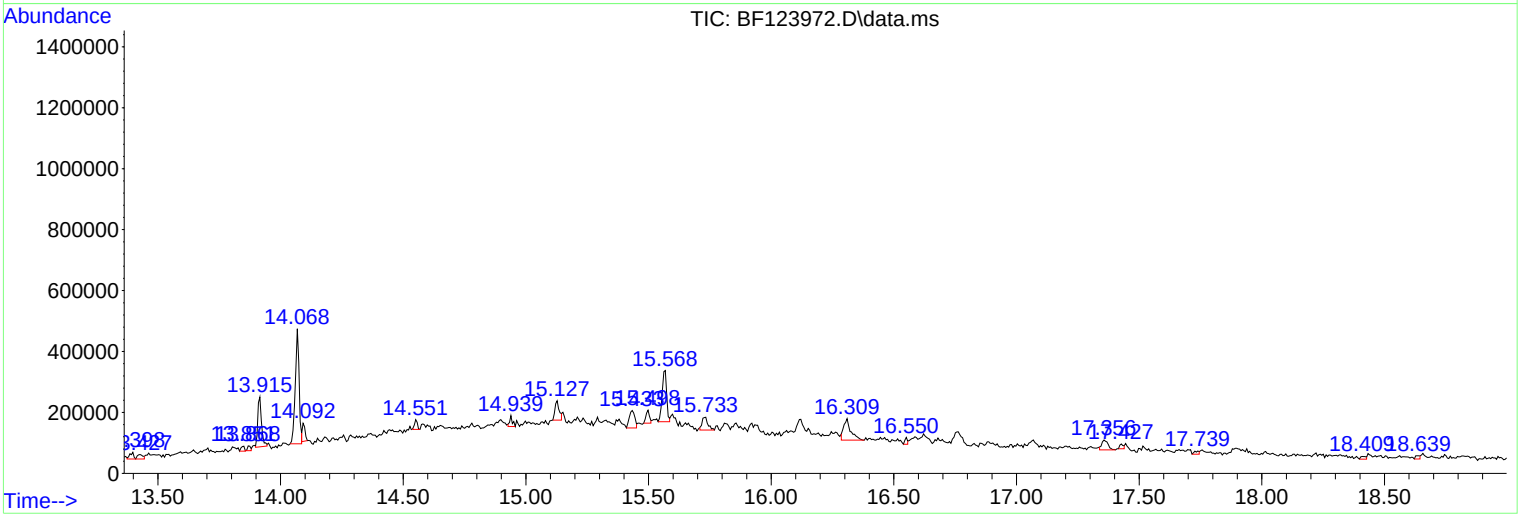
Instrument :
BNA_F
ClientSampleId :
SB-08-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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Data File : BF123972.D
Acq On : 17 May 2021 19:54
Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-COMP

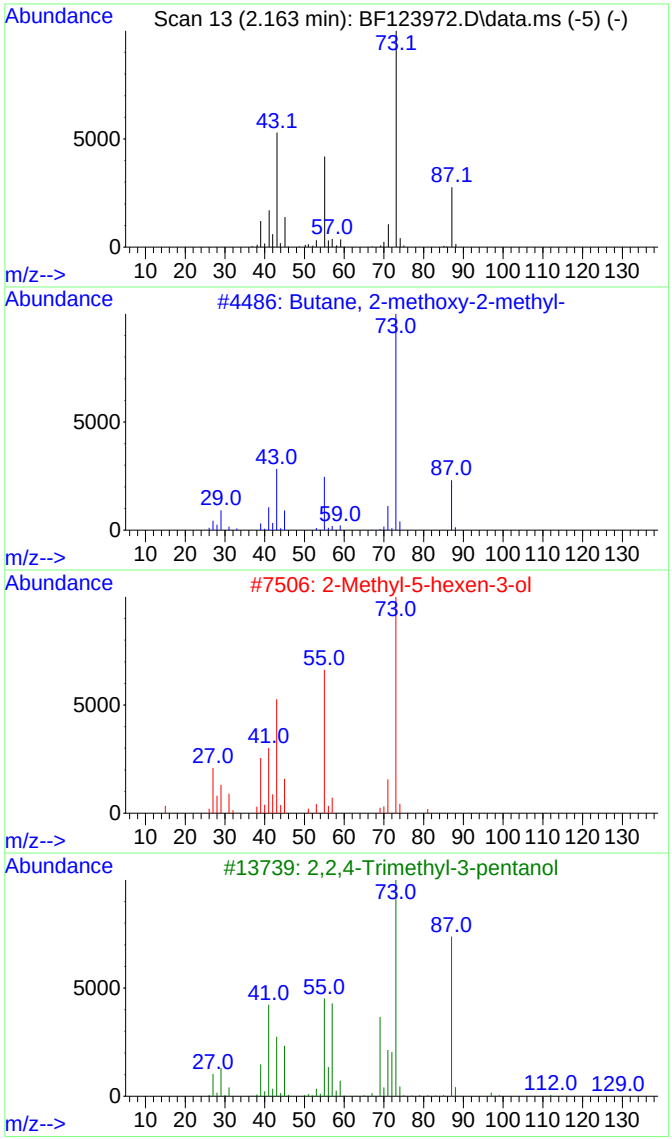
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

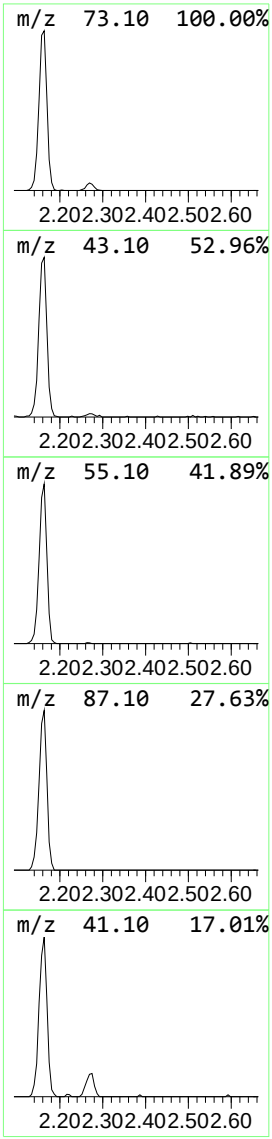
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	47.93 ng	617207	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-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123972.D
Acq On : 17 May 2021 19:54
Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

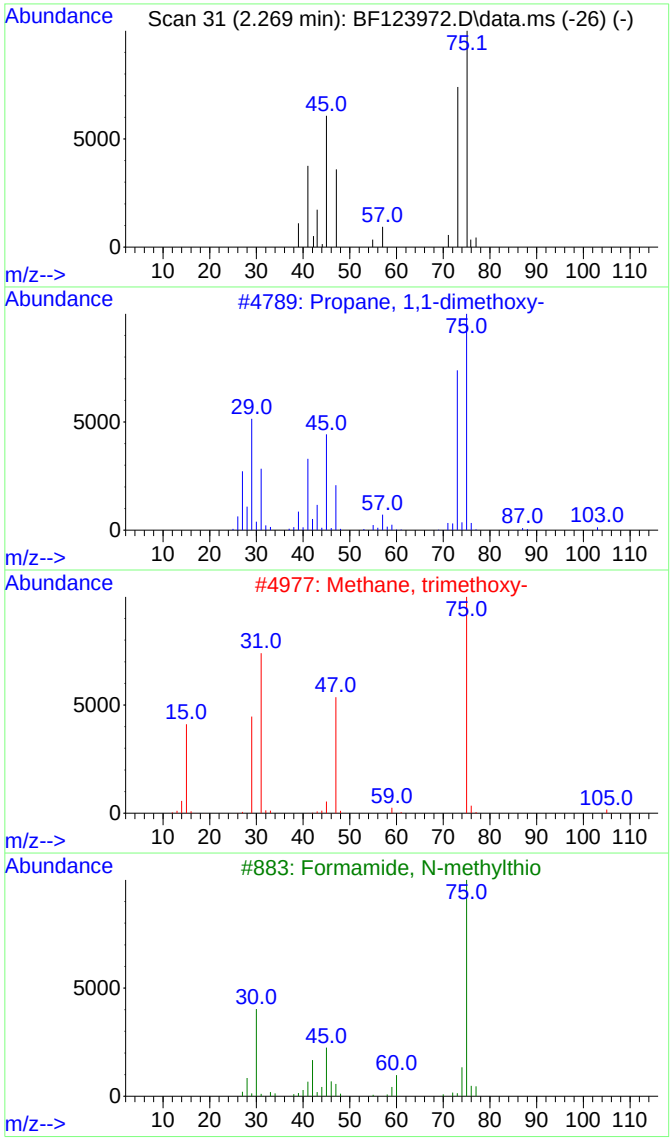
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

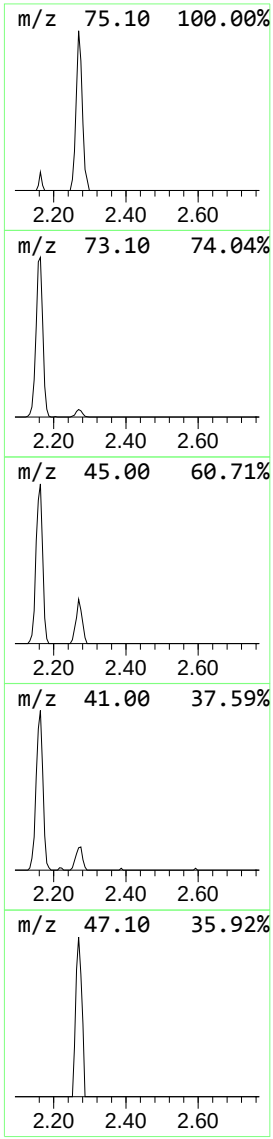
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.269	3.48 ng	44842	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Methane, trimethoxy-	106	C4H10O3	000149-73-5	9
3	Formamide, N-methylthio	75	C2H5NS	018952-41-5	5
4	Ethanethioamide	75	C2H5NS	000062-55-5	5
5	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123972.D
Acq On : 17 May 2021 19:54
Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

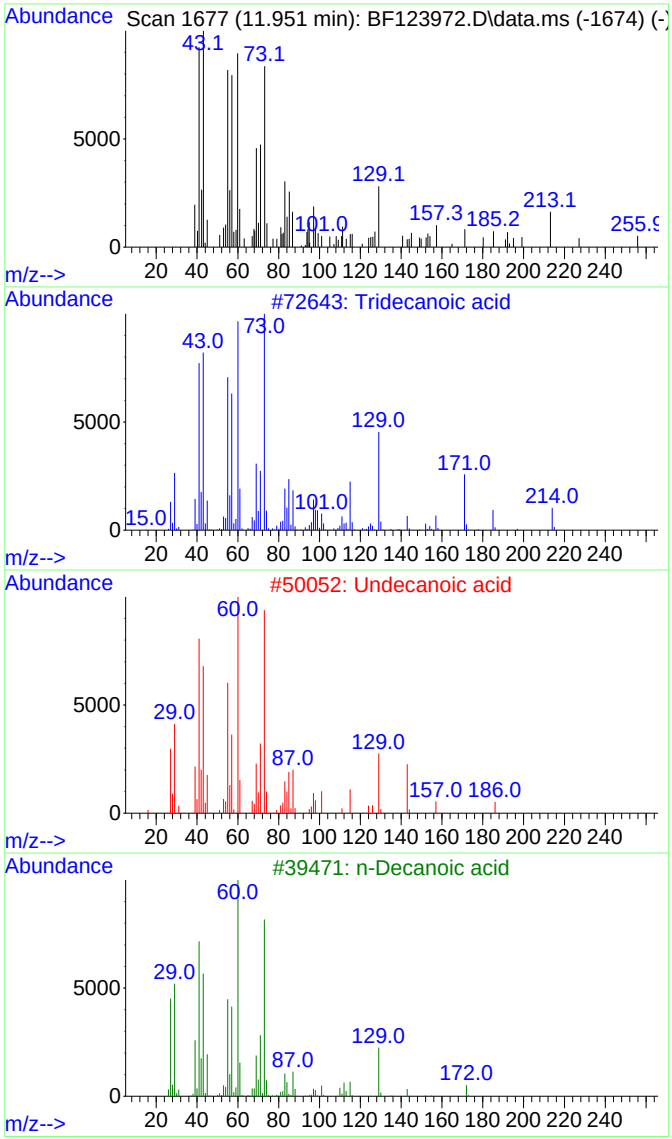
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

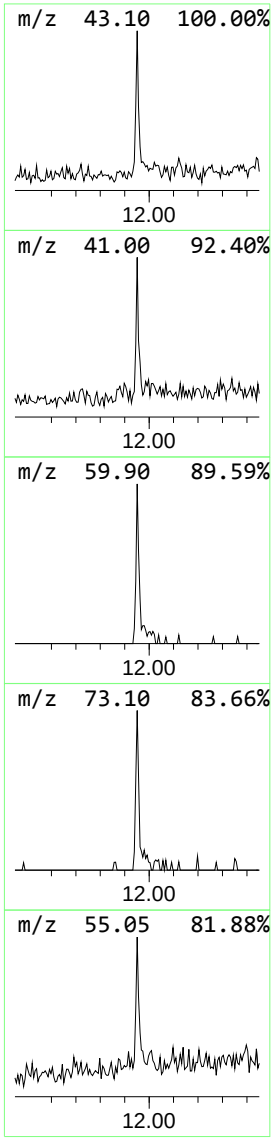
****

Peak Number 3 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	4.73 ng	83509	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	59
2	Undecanoic acid	186	C11H22O2	000112-37-8	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	43
5	Oxalic acid, propyl tridecyl ester	314	C18H34O4	1000309-26-6	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123972.D
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Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

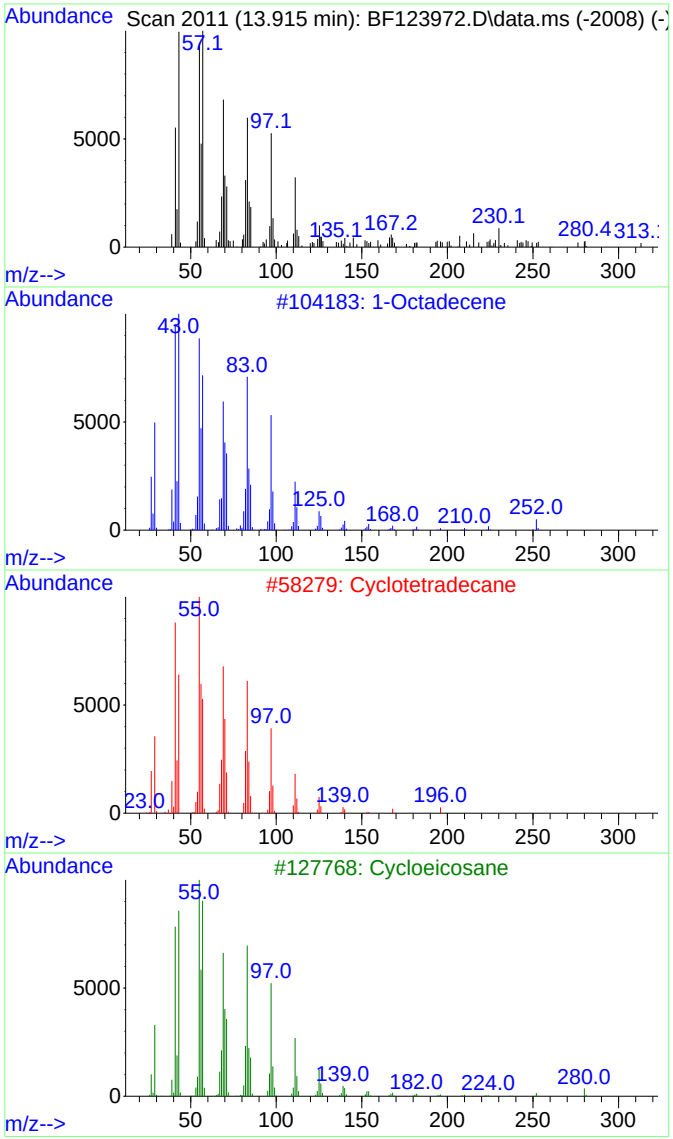
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

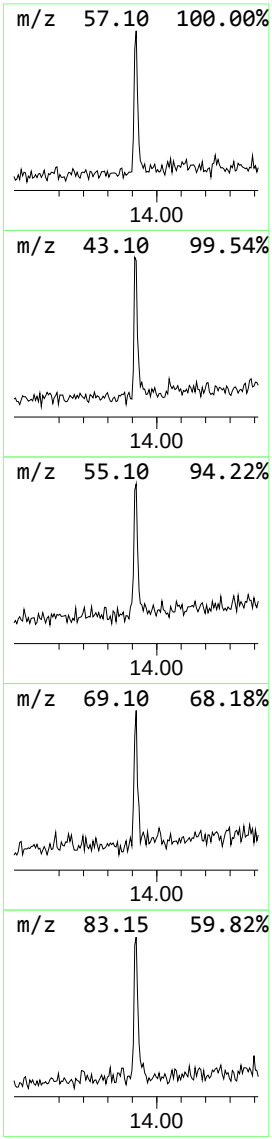
****

Peak Number 4 1-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.915	8.40 ng	174105	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	97
2	Cyclotetradecane	196	C14H28	000295-17-0	96
3	Cycloeicosane	280	C20H40	000296-56-0	96
4	Cetene	224	C16H32	000629-73-2	94
5	1-Eicosene	280	C20H40	003452-07-1	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123972.D
Acq On : 17 May 2021 19:54
Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

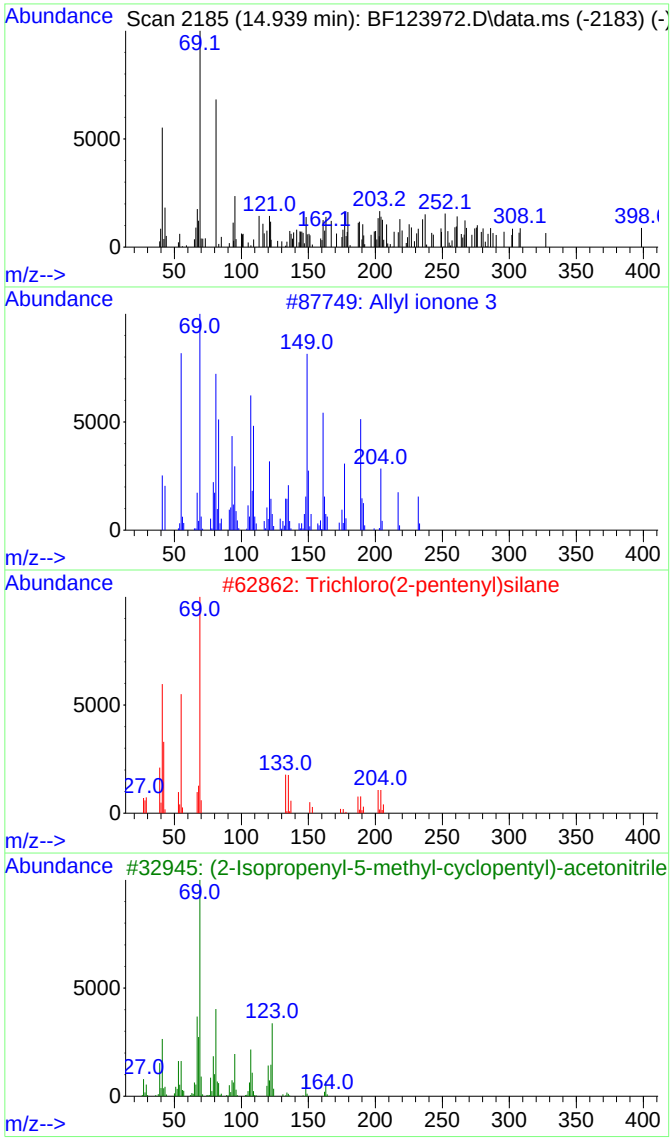
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

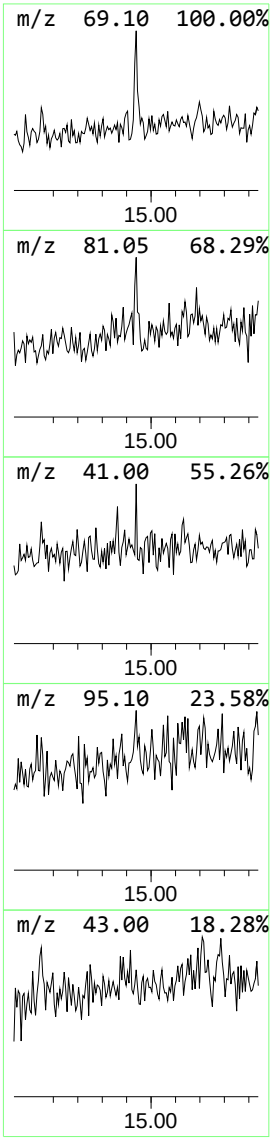
****

Peak Number 5 unknown14.939 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	2.41 ng	25909	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allyl ionone 3	232	C16H24O	1000284-92-9	46
2	Trichloro(2-pentenyl)silane	202	C5H9Cl3Si	1000109-99-7	41
3	(2-Isopropenyl-5-methyl-cyclopen...	163	C11H17N	1000193-43-9	38
4	2-Hexene, 6-iodo-2-methyl-	224	C7H13I	063588-94-3	35
5	Diazene, 1-cyclopentyl-2-methoxy...	144	C6H12N2O2	108201-44-1	35





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Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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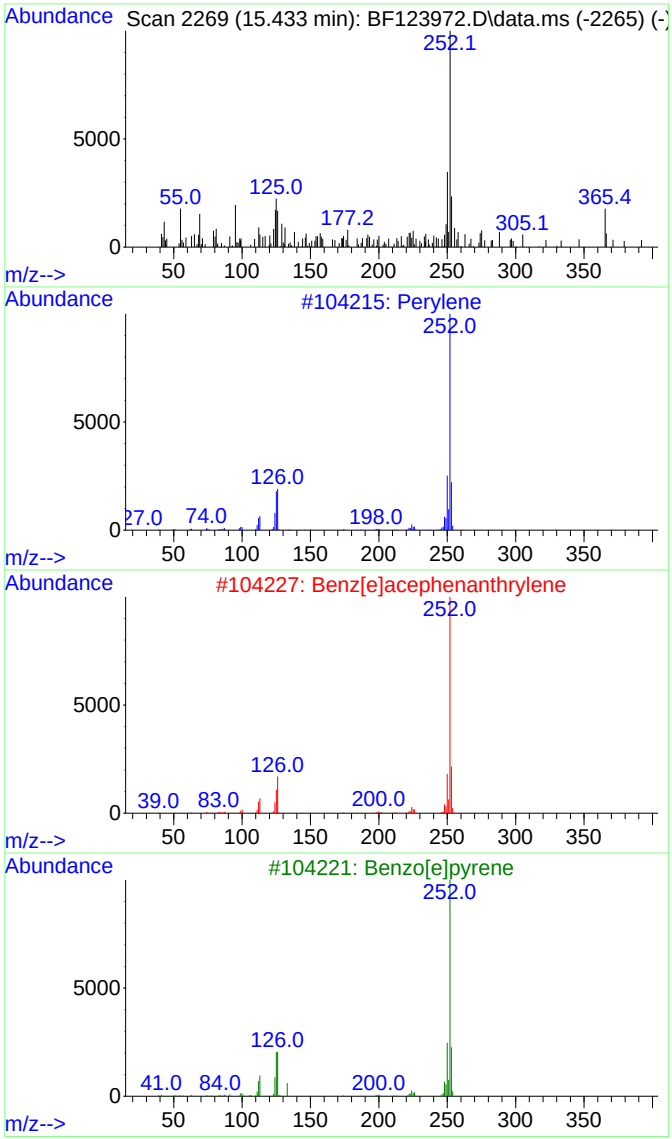
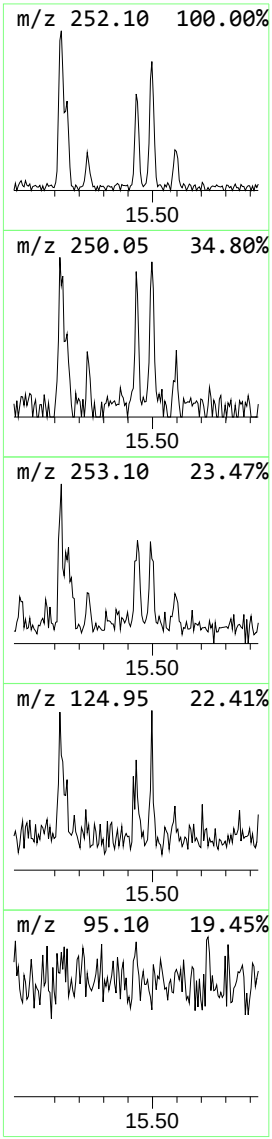
Peak Number 6 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.433	8.40 ng	90287	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	58
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	55
3	Benzo[e]pyrene	252	C20H12	000192-97-2	52
4	8-Chloro-11H-indolo[3,2-c]quinoline	252	C15H9ClN2	155249-69-7	47
5	Benzo[a]pyrene	252	C20H12	000050-32-8	47





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Data File : BF123972.D
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Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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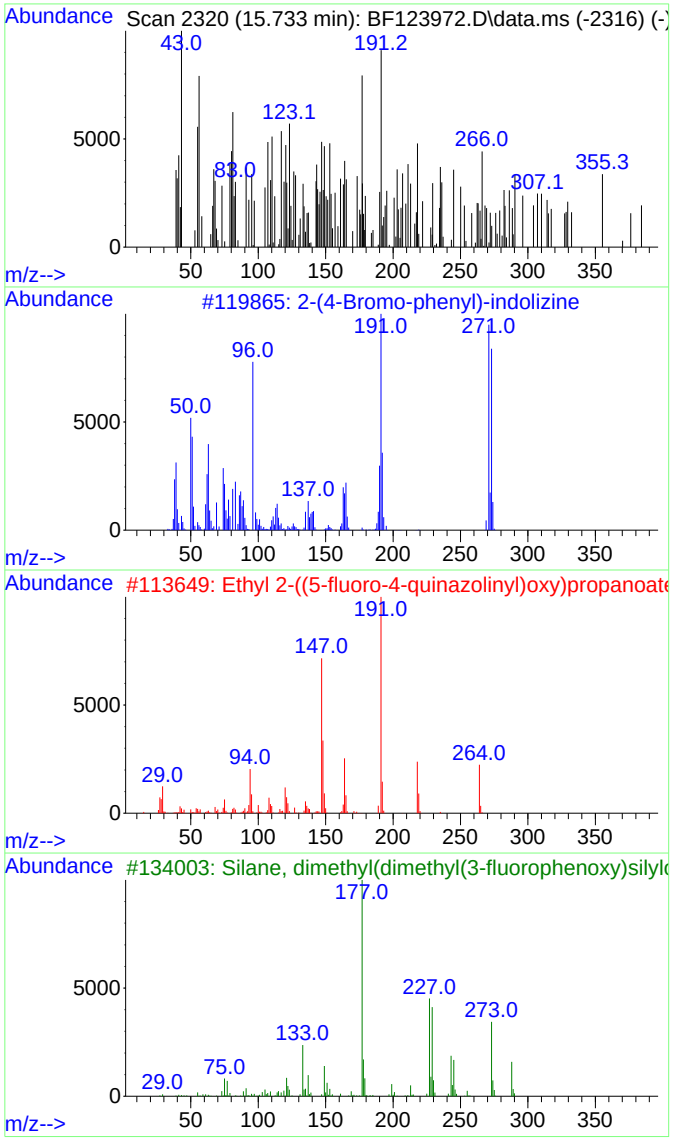
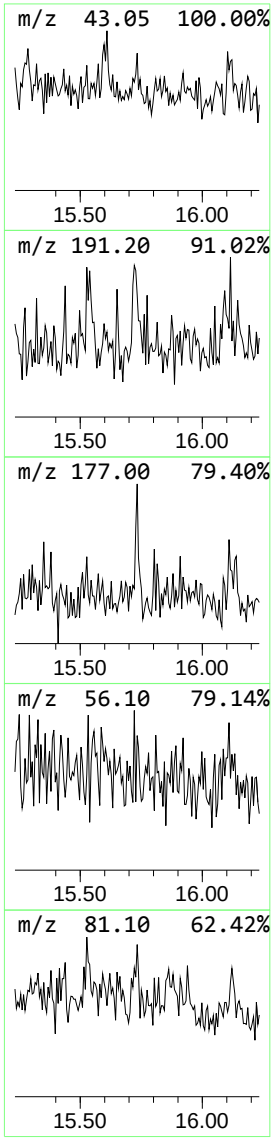
Peak Number 7 unknown15.733 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	6.33 ng	68049	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Bromo-phenyl)-indolizine	271	C14H10BrN	007496-72-2	25
2	Ethyl 2-((5-fluoro-4-quinazoliny...	264	C13H13FN2O3	1000332-11-2	25
3	Silane, dimethyl(dimethyl(3-fluo...	288	C12H21FO3Si2	1000347-39-4	15
4	N-[4-(Acetylamino)tricyclo[3.3.1...	250	C14H22N2O2	1000305-58-9	15
5	2-Methyl-7,7,8,8-tetracyano-p-qu...	218	C13H6N4	001518-13-4	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123972.D
Acq On : 17 May 2021 19:54
Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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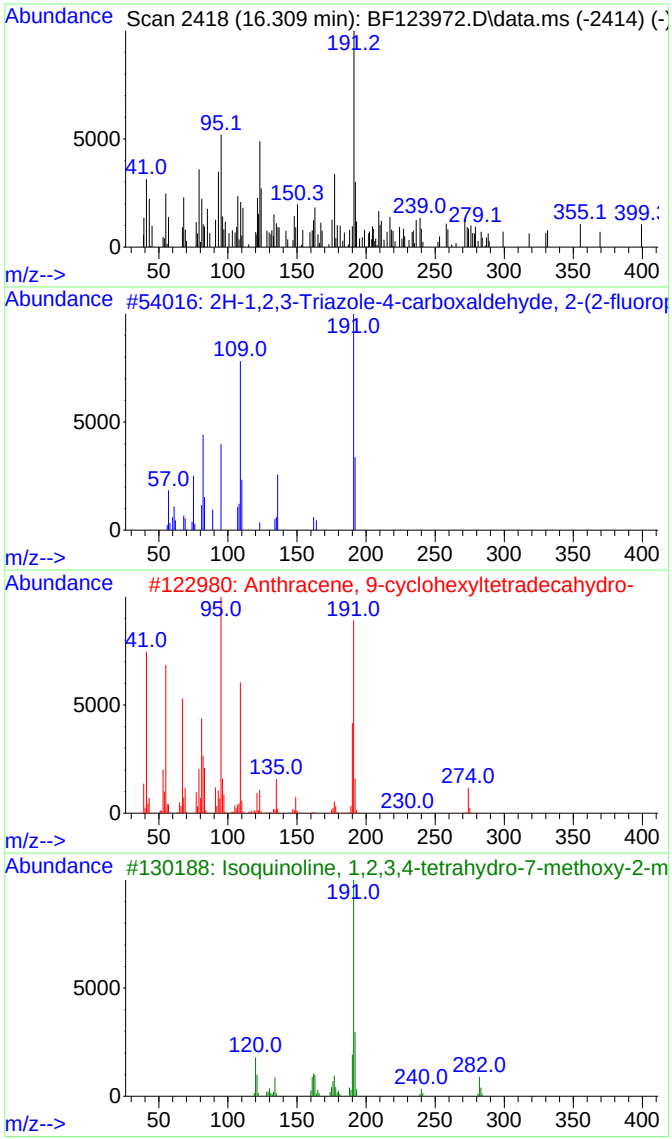
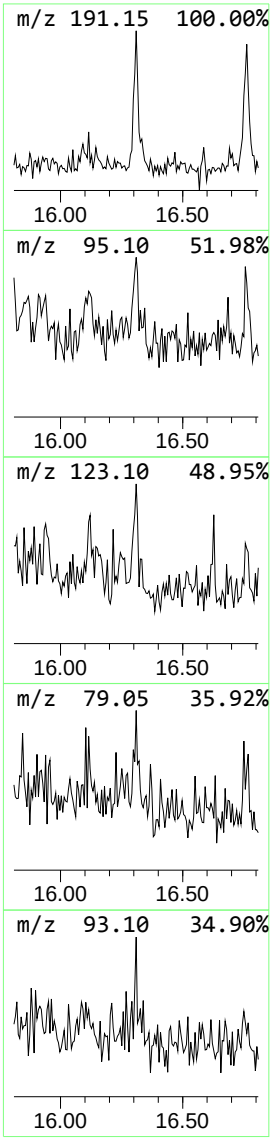
Peak Number 8 unknown16.309 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.309	12.89 ng	138520	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	47
2	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	46
3	Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21NO2	036646-87-4	43
4	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	35
5	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123972.D
Acq On : 17 May 2021 19:54
Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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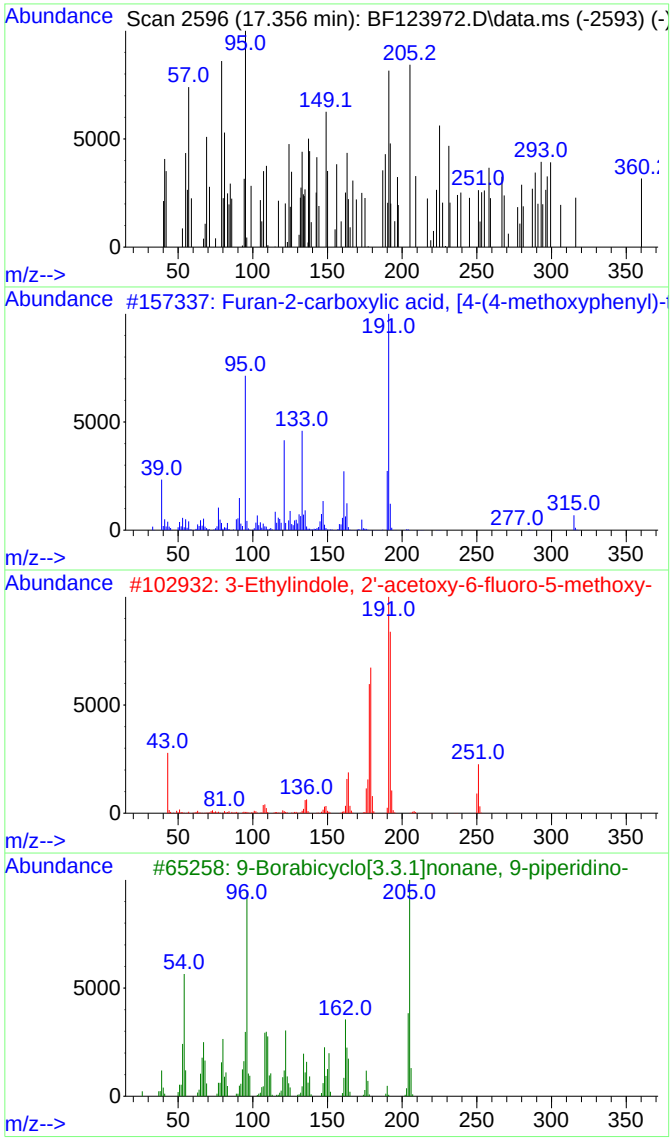
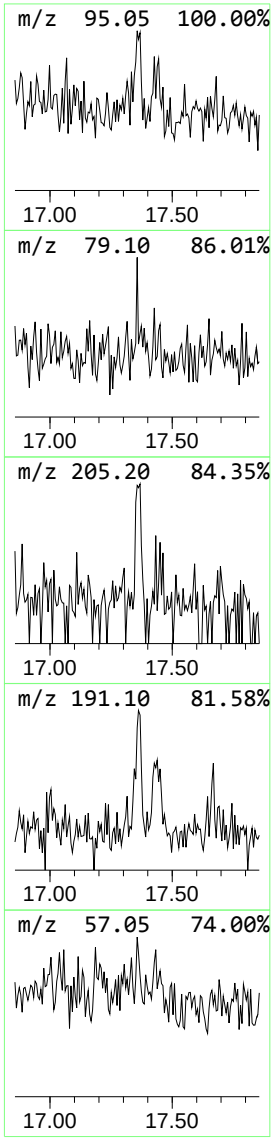
Peak Number 9 unknown17.356 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.356	5.21 ng	55942	Perylene-d12	15.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan-2-carboxylic acid, [4-(4-m...	315	C18H21NO4	1000305-72-3	12
2	3-Ethylindole, 2'-acetoxy-6-fluo...	251	C13H14FNO3	1000116-27-7	10
3	9-Borabicyclo[3.3.1]nonane, 9-pi...	205	C13H24BN	022516-42-3	10
4	2-Hydroxy-4-methyl-6-(2-thienyl)...	192	C9H8N2OS	026963-45-1	10
5	1,3-Cyclohexanedione, 2-(ethoxym...	280	C15H20O5	029817-43-4	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123972.D
Acq On : 17 May 2021 19:54
Operator : JU/CG
Sample : M2392-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-08-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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...	2.163	47.9	ng	617207	1	6.904	257557	20.0
Propane, 1,1-di...	2.269	3.5	ng	44842	1	6.904	257557	20.0
Tridecanoic acid	11.951	4.7	ng	83509	4	11.427	352990	20.0
1-Octadecene	13.915	8.4	ng	174105	5	14.068	414351	20.0
unknown14.939	14.939	2.4	ng	25909	6	15.562	214879	20.0
Perylene	15.433	8.4	ng	90287	6	15.562	214879	20.0
unknown15.733	15.733	6.3	ng	68049	6	15.562	214879	20.0
unknown16.309	16.309	12.9	ng	138520	6	15.562	214879	20.0
unknown17.356	17.356	5.2	ng	55942	6	15.562	214879	20.0