LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052021\
Data File : BF124010.D
Acq On : 20 May 2021 15:39
Operator : JU/CG
Sample : M2468-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-5-TP

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: BF124010.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	14	rVB	226498	293407	43.51%	3.910%
2	2.252	24	28	33	rVB2	17090	23786	3.53%	0.317%
3	5.104	510	513	522	rVB	56153	61989	9.19%	0.826%
4	5.516	578	583	586	rBV	576894	508291	75.38%	6.774%
5	6.522	750	754	761	rBV	626369	531962	78.89%	7.089%
6	6.904	816	819	823	rBV	450988	343537	50.94%	4.578%
7	7.463	910	914	917	rBV	480300	367266	54.46%	4.894%
8	8.192	1034	1038	1041	rBV	528180	449366	66.64%	5.988%
9	9.263	1217	1220	1223	rBV	906301	674345	100.00%	8.986%
10	9.381	1236	1240	1243	rBV	24158	20532	3.04%	0.274%
11	9.657	1283	1287	1292	rBV	20721	18486	2.74%	0.246%
12	9.945	1332	1336	1346	rBV	666198	555282	82.34%	7.400%
13	10.733	1466	1470	1480	rBV	460585	451382	66.94%	6.015%
14	10.916	1497	1501	1503	rBV2	9107	8752	1.30%	0.117%
15	10.945	1503	1506	1509	rVB2	8086	9426	1.40%	0.126%
16	11.092	1528	1531	1534	rBV3	7854	8642	1.28%	0.115%
17	11.310	1561	1568	1569	rBV3	5799	10596	1.57%	0.141%
18	11.433	1585	1589	1592	rBV	628323	527848	78.28%	7.034%
19	11.457	1592	1593	1596	rVB	34549	18662	2.77%	0.249%
20	11.651	1622	1626	1630	rBV3	5604	10446	1.55%	0.139%
21	11.951	1672	1677	1682	rBV5	45013	63084	9.35%	0.841%
22	12.045	1690	1693	1696	rBV3	11098	11764	1.74%	0.157%
23	12.251	1726	1728	1731	rBV3	9544	8688	1.29%	0.116%
24	12.645	1792	1795	1799	rBV	83912	76450	11.34%	1.019%
25	12.739	1808	1811	1814	rBV6	15131	14569	2.16%	0.194%
26	12.874	1831	1834	1836	rBV	64074	46755	6.93%	0.623%
27	13.016	1854	1858	1861	rBV	773791	630850	93.55%	8.407%
28	13.104	1869	1873	1874	rBV4	8728	10895	1.62%	0.145%
29	13.151	1878	1881	1884	rVB5	8701	10442	1.55%	0.139%
30	13.710	1973	1976	1981	rBV7	18788	18438	2.73%	0.246%
31	13.851	1991	2000	2008	rBV7	63844	257197	38.14%	3.427%
32	13.916	2008	2011	2017	rVB	149436	168003	24.91%	2.239%
33	14.074	2033	2038	2041	rBV	465417	460715	68.32%	6.140%
34	14.239	2063	2066	2068	rBV4	20965	16940	2.51%	0.226%
35	14.410	2090	2095	2096	rBV5	21605	32161	4.77%	0.429%
36	14.439	2096	2100	2102	rVV5	18199	25813	3.83%	0.344%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052021\
Data File : BF124010.D
Acq On : 20 May 2021 15:39
Operator : JU/CG
Sample : M2468-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-5-TP

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	14.557	2116	2120	2125	rVB7	42708	80701	11.97%	1.075%
38	15.010	2195	2197	2199	rVB3	26695	22315	3.31%	0.297%
39	15.098	2210	2212	2213	rBV2	15604	8760	1.30%	0.117%
40	15.127	2215	2217	2220	rVV4	23663	33711	5.00%	0.449%
41	15.210	2228	2231	2233	rBV2	33780	38712	5.74%	0.516%
42	15.568	2288	2292	2297	rBV	212513	287642	42.66%	3.833%
43	16.057	2372	2375	2379	rVB3	60395	78356	11.62%	1.044%
44	16.115	2383	2385	2392	rVB8	34837	64685	9.59%	0.862%
45	16.310	2416	2418	2422	rVB5	16047	12815	1.90%	0.171%
46	17.609	2637	2639	2641	rBV3	12239	8976	1.33%	0.120%
47	17.657	2645	2647	2648	rBV2	13031	10219	1.52%	0.136%
48	17.709	2651	2656	2661	rBV9	34272	71713	10.63%	0.956%
49	17.927	2691	2693	2695	rBV3	16391	14906	2.21%	0.199%
50	17.998	2703	2705	2708	rBV4	11902	8947	1.33%	0.119%
51	18.298	2753	2756	2757	rBV3	12298	14827	2.20%	0.198%

Sum of corrected areas: 7504052

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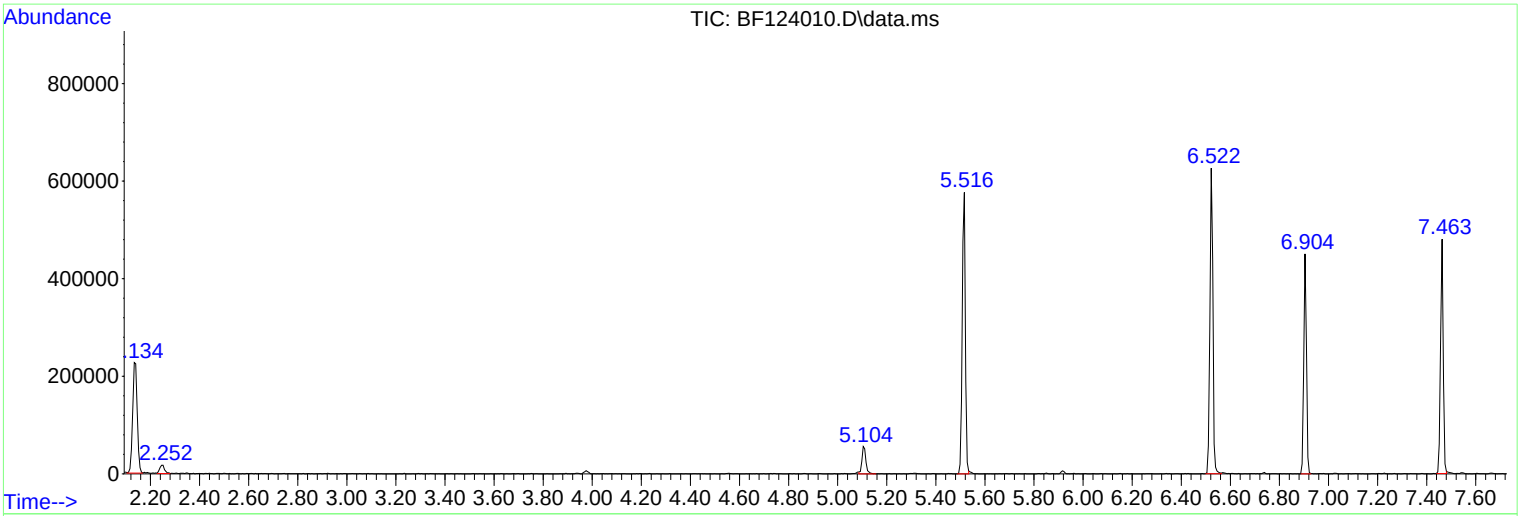
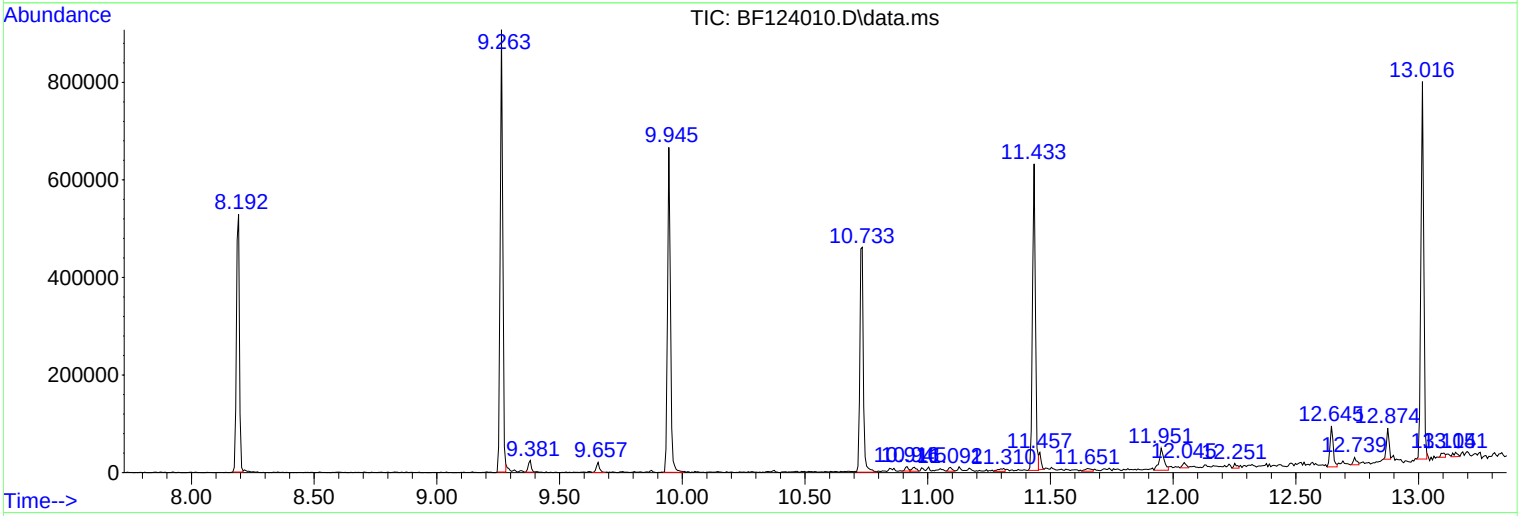
ALS Vial : 10 Sample Multiplier: 1

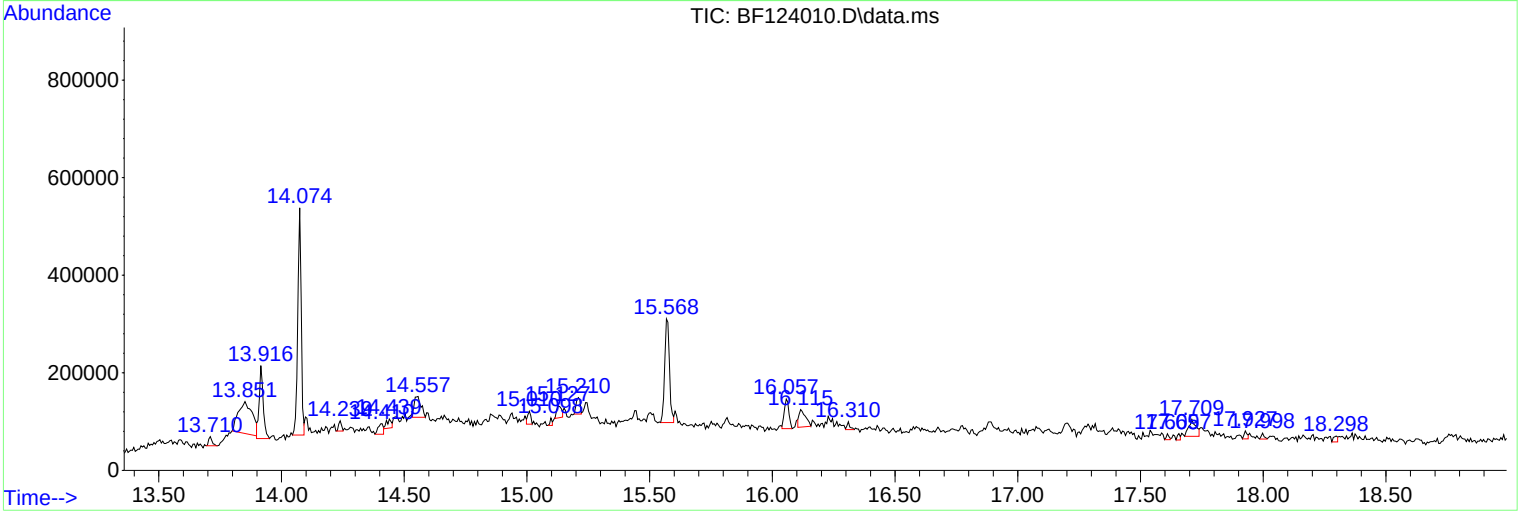
Instrument :
BNA_F
ClientSampleId :
1-5-TP

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

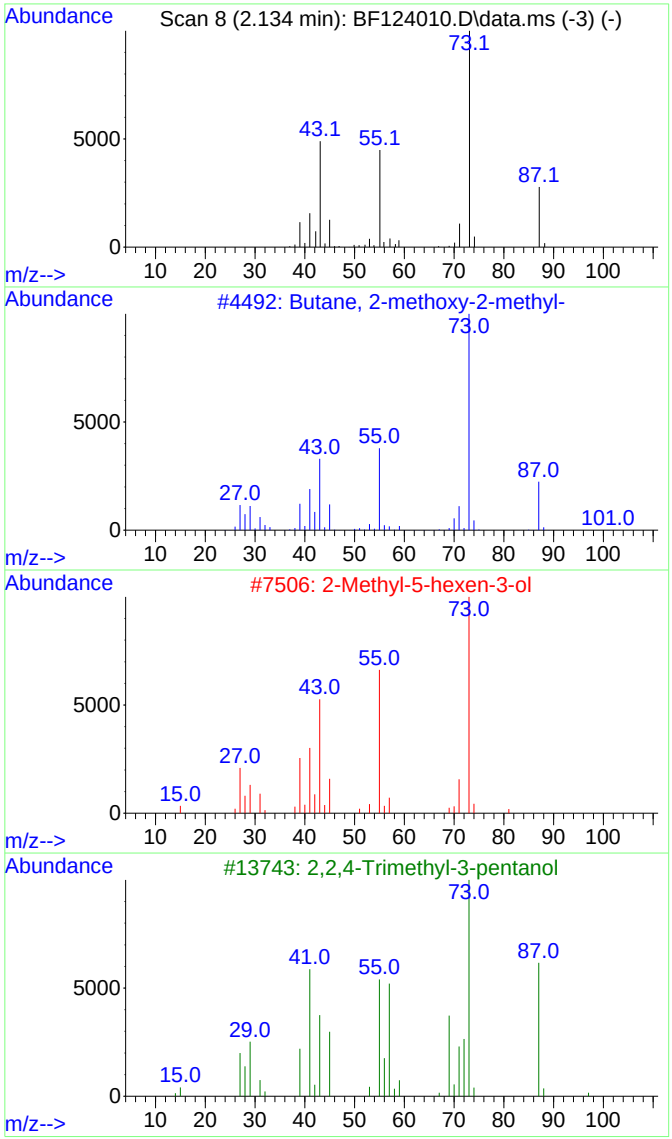
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

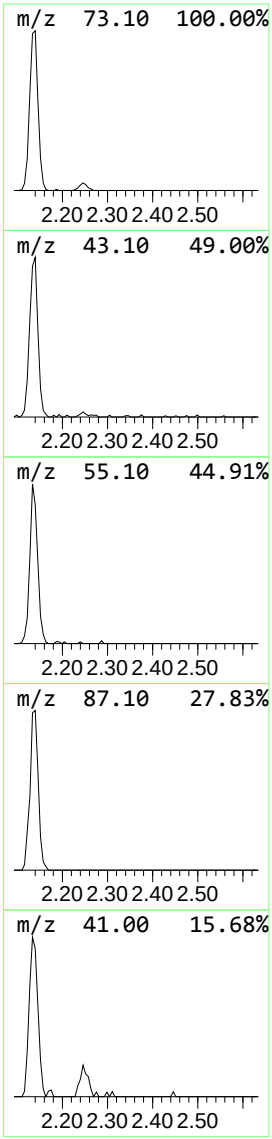
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	17.08 ng	293407	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	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	47
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	33
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23





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Sample : M2468-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-5-TP

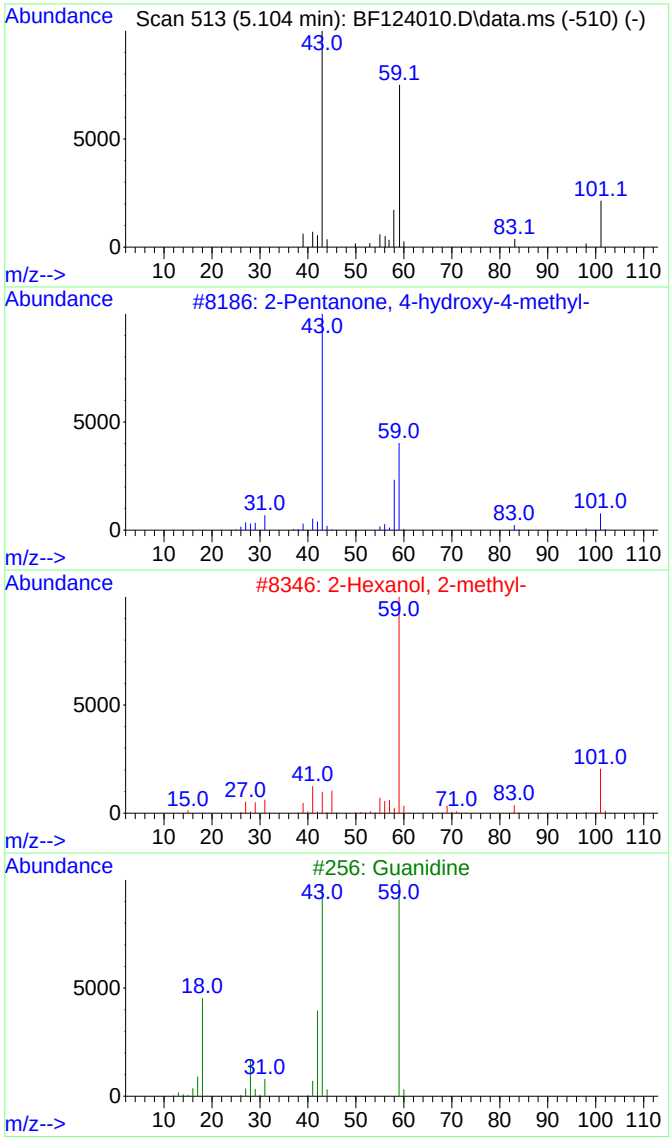
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

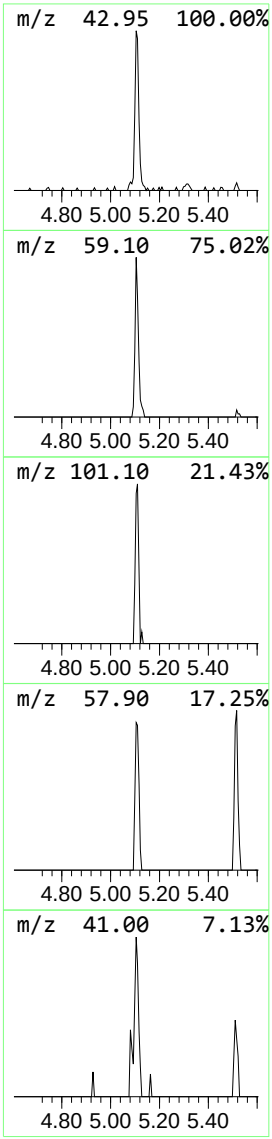
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	3.61 ng	61989	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	59
3	Guanidine	59	CH5N3	000113-00-8	53
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	40
5	3-Hexanol	102	C6H14O	000623-37-0	36





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Acq On : 20 May 2021 15:39
Operator : JU/CG
Sample : M2468-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-5-TP

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

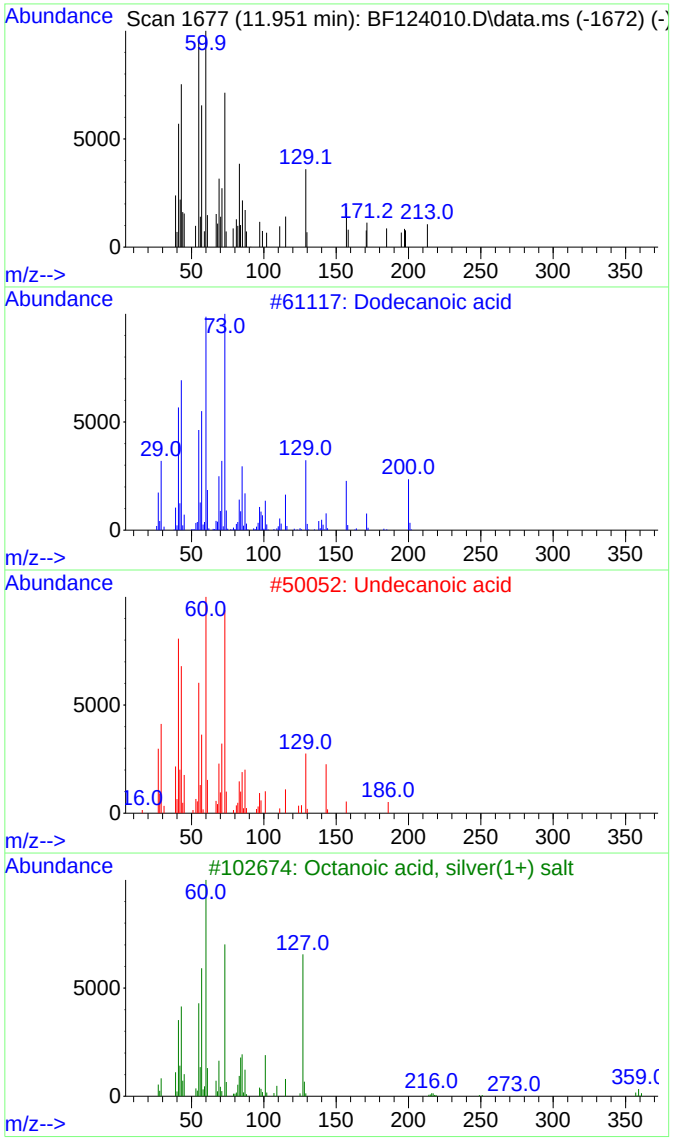
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

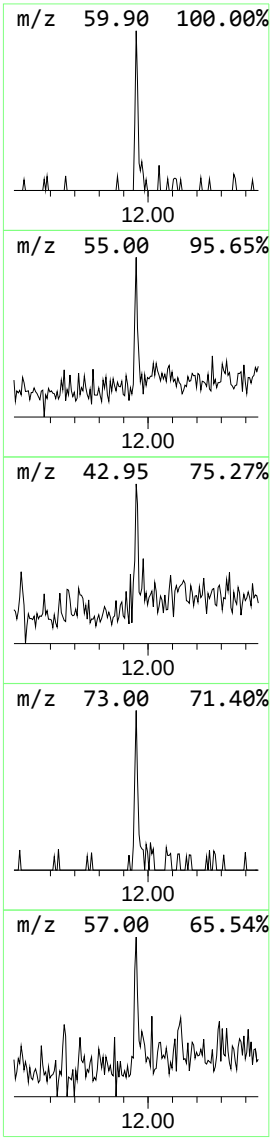
****

Peak Number 3 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.39 ng	63084	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	58
2	Undecanoic acid	186	C11H22O2	000112-37-8	47
3	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	38
4	n-Decanoic acid	172	C10H20O2	000334-48-5	35
5	Nonanoic acid	158	C9H18O2	000112-05-0	35





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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-5-TP

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

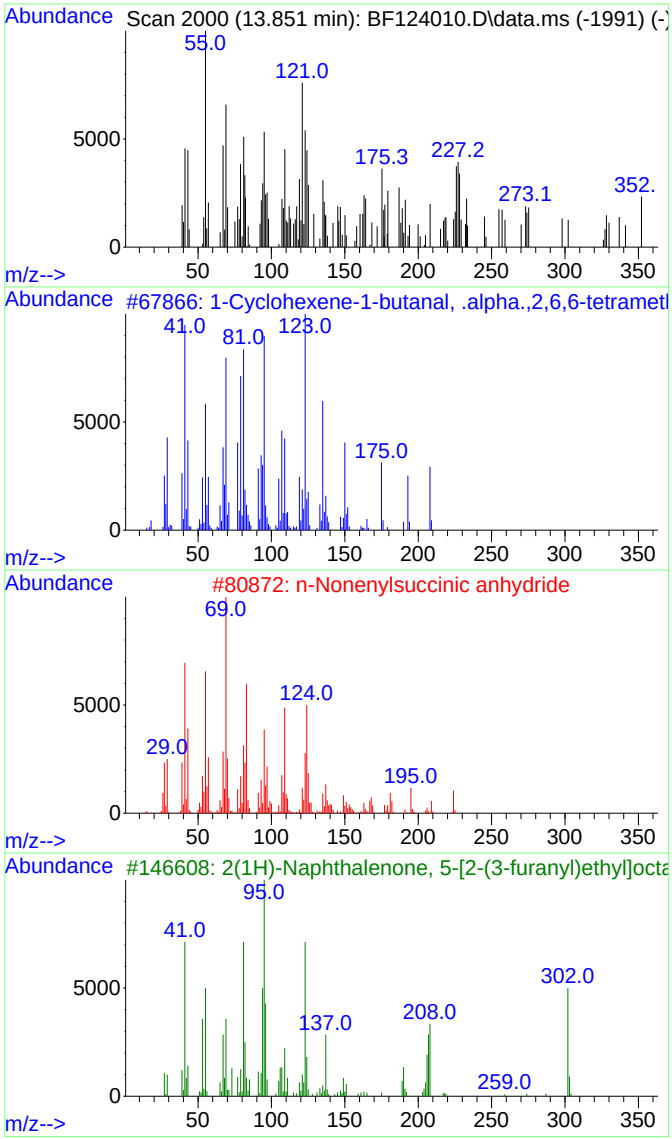
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

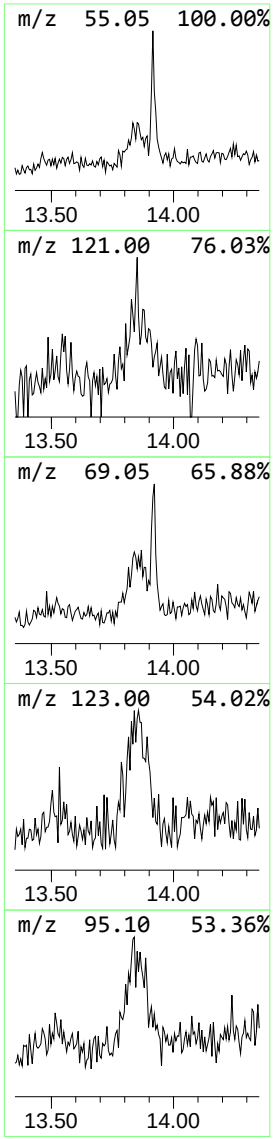
****

Peak Number 5 unknown13.85 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	11.17 ng	257197	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexene-1-butanal, .alpha....	208	C14H24O	021632-06-4	35
2	n-Nonenylsuccinic anhydride	224	C13H20O3	028928-97-4	30
3	2(1H)-Naphthalenone, 5-[2-(3-fur...	302	C20H30O2	059742-40-4	30
4	Benzamide, 2-fluoro-N-(2-methoxy...	259	C15H14FNO2	331270-36-1	22
5	Benzaldehyde, 4-fluoro-	124	C7H5FO	000459-57-4	22





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Instrument :
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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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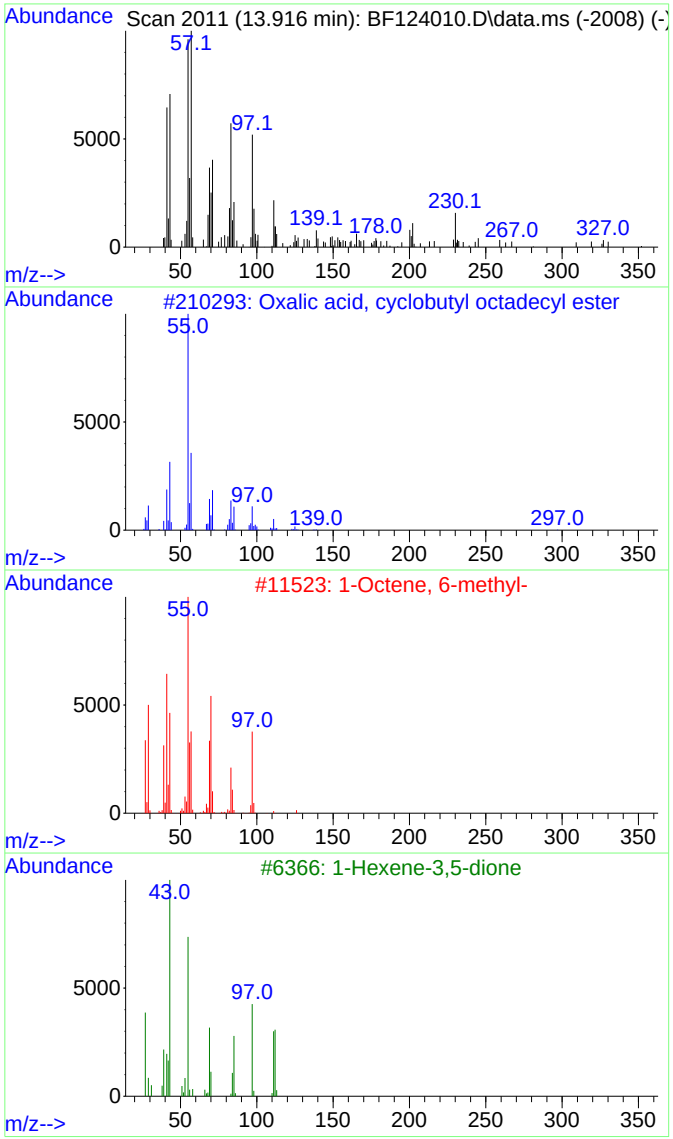
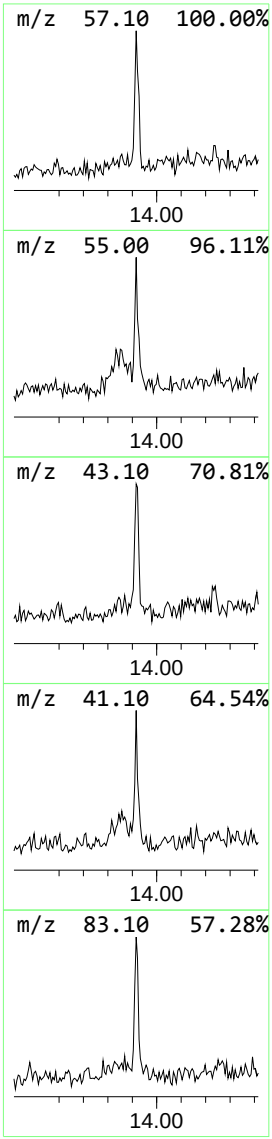
****
Peak Number 6 unknown13.91 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	7.29 ng	168003	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	38
2	1-Octene, 6-methyl-	126	C9H18	013151-10-5	25
3	1-Hexene-3,5-dione	112	C6H8O2	052204-69-0	25
4	Undecane	156	C11H24	001120-21-4	20
5	3-Heptene, 5-methyl-	112	C8H16	013172-91-3	18





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ALS Vial : 10 Sample Multiplier: 1

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

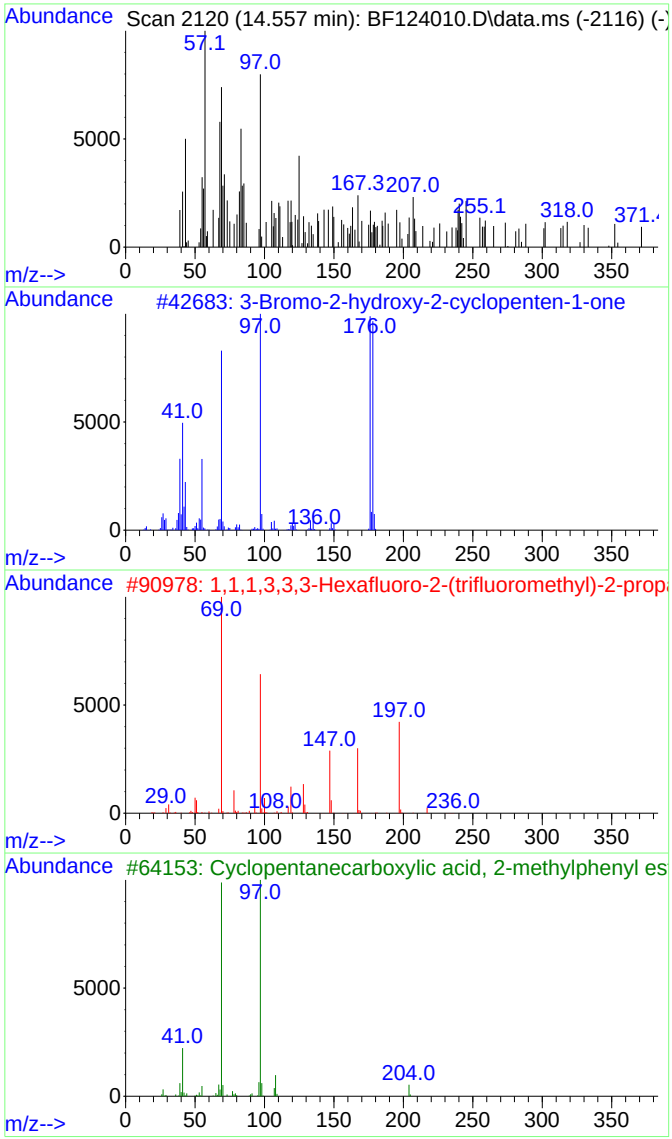
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

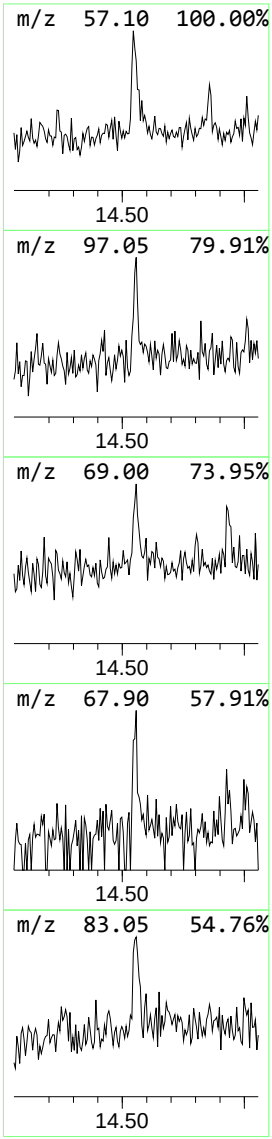
****

Peak Number 7 unknown14.55 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	3.50 ng	80701	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Bromo-2-hydroxy-2-cyclopenten-...	176	C5H5BrO2	003019-83-8	43
2	1,1,1,3,3,3-Hexafluoro-2-(triflu...	236	C4HF9O	002378-02-1	43
3	Cyclopentanecarboxylic acid, 2-m...	204	C13H16O2	055229-43-1	43
4	6-Bromo-2,2-dimethylcyclohexanone	204	C8H13BrO	021690-26-6	43
5	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	43





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Misc :
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Instrument : BNA_F
ClientSampleId : 1-5-TP

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

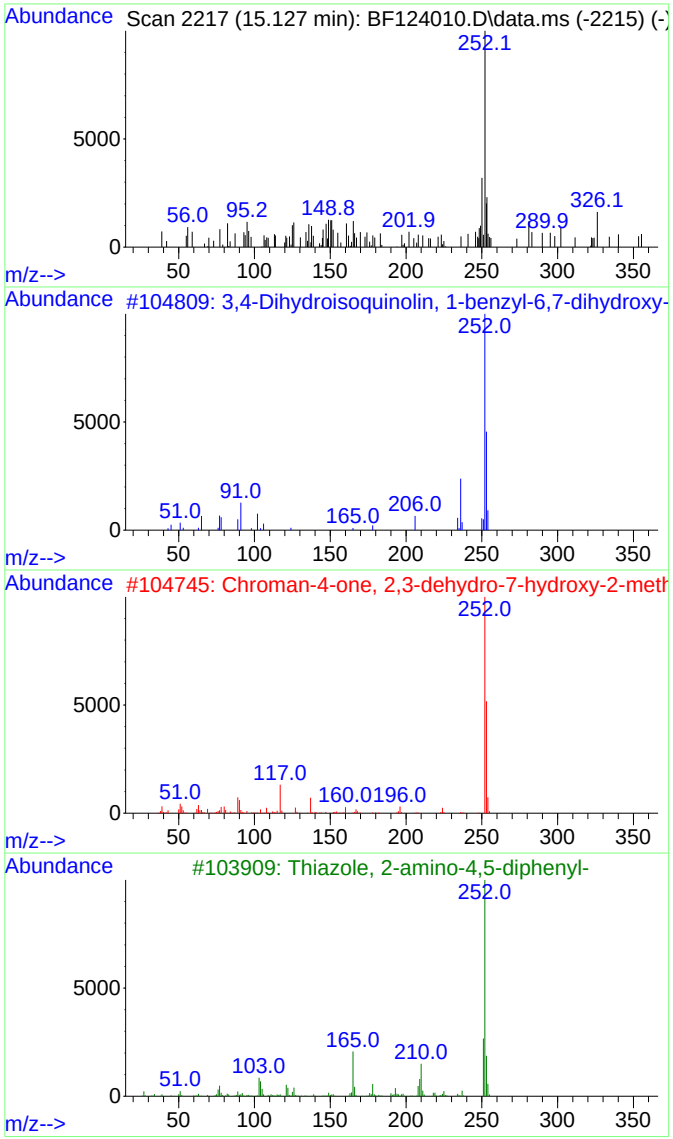
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

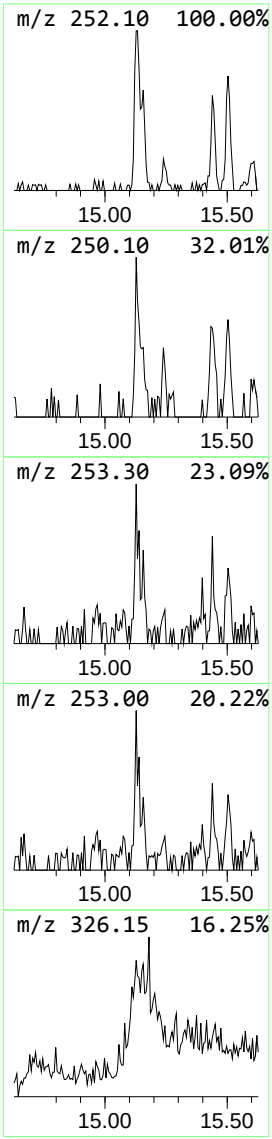
****

Peak Number 8 unknown15.12 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.34 ng	33711	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dihydroisoquinolin, 1-benzyl...	253	C16H15NO2	017578-74-4	47
2	Chroman-4-one, 2,3-dehydro-7-hyd...	253	C15H11NO3	065047-28-1	47
3	Thiazole, 2-amino-4,5-diphenyl-	252	C15H12N2S	006318-74-7	38
4	12H-[1,3]Benzothiazolo[2,3-b]qui...	252	C14H8N2OS	1000338-32-6	35
5	1-Formyl-4-hydroxyanthraquinone	252	C15H8O4	092011-74-0	35





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

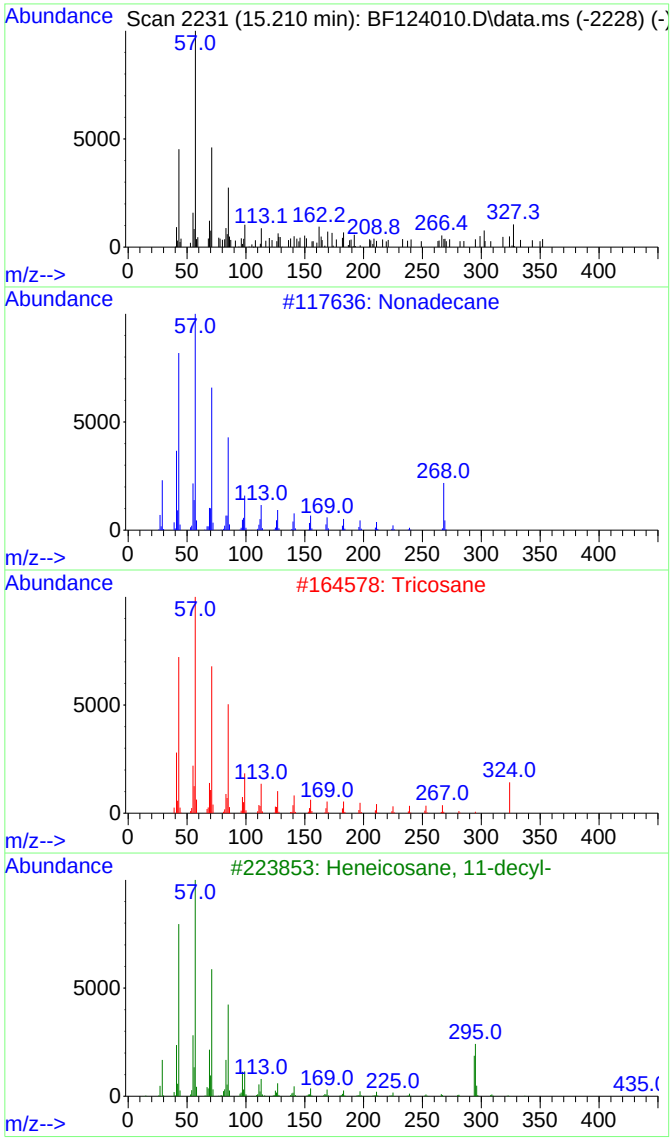
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

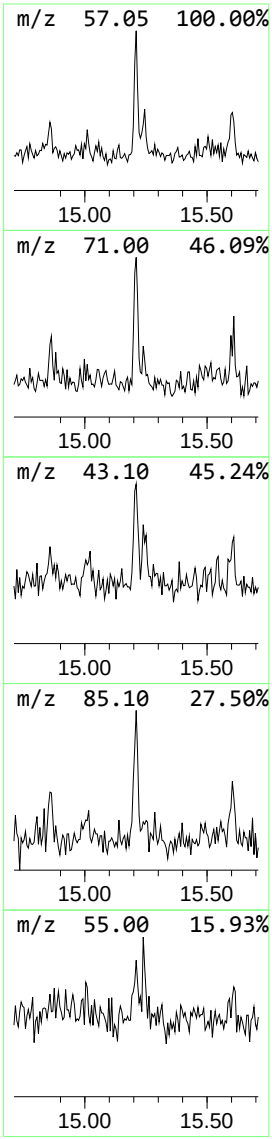
****

Peak Number 9 unknown15.21 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	2.69 ng	38712	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	47
2	Tricosane	324	C23H48	000638-67-5	47
3	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	43
4	Eicosane, 10-hexyl-10-methyl-	380	C27H56	055282-32-1	37
5	3,3,13,13-Tetraethylpentadecane	324	C23H48	1000360-42-3	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052021\
Data File : BF124010.D
Acq On : 20 May 2021 15:39
Operator : JU/CG
Sample : M2468-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-5-TP

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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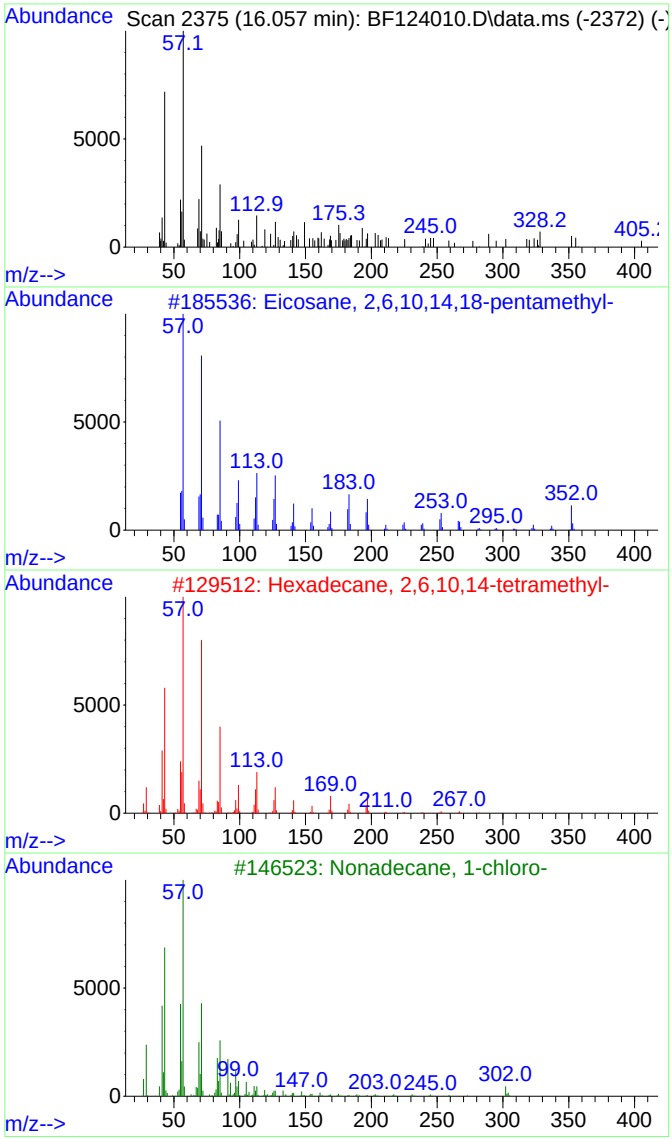
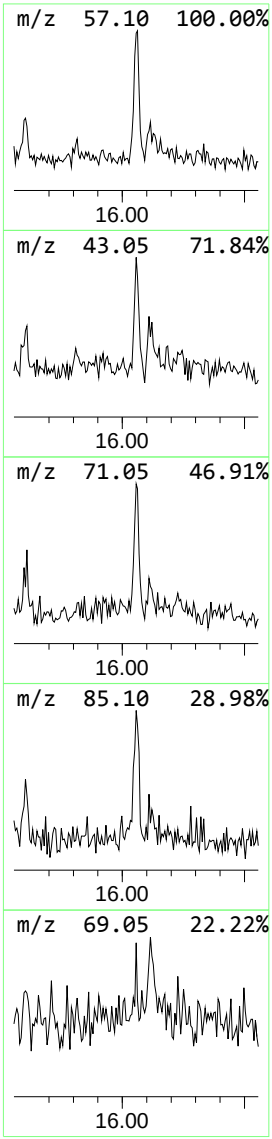
Peak Number 10 Eicosane, 2,6,10,14,18-pent... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.057	5.45 ng	78356	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 2,6,10,14,18-pentamethyl-	352	C25H52	051794-16-2	70
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	60
3	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	52
4	Nonadecane, 4-methyl-	282	C20H42	025117-27-5	49
5	Tridecane	184	C13H28	000629-50-5	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052021\
Data File : BF124010.D
Acq On : 20 May 2021 15:39
Operator : JU/CG
Sample : M2468-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-5-TP

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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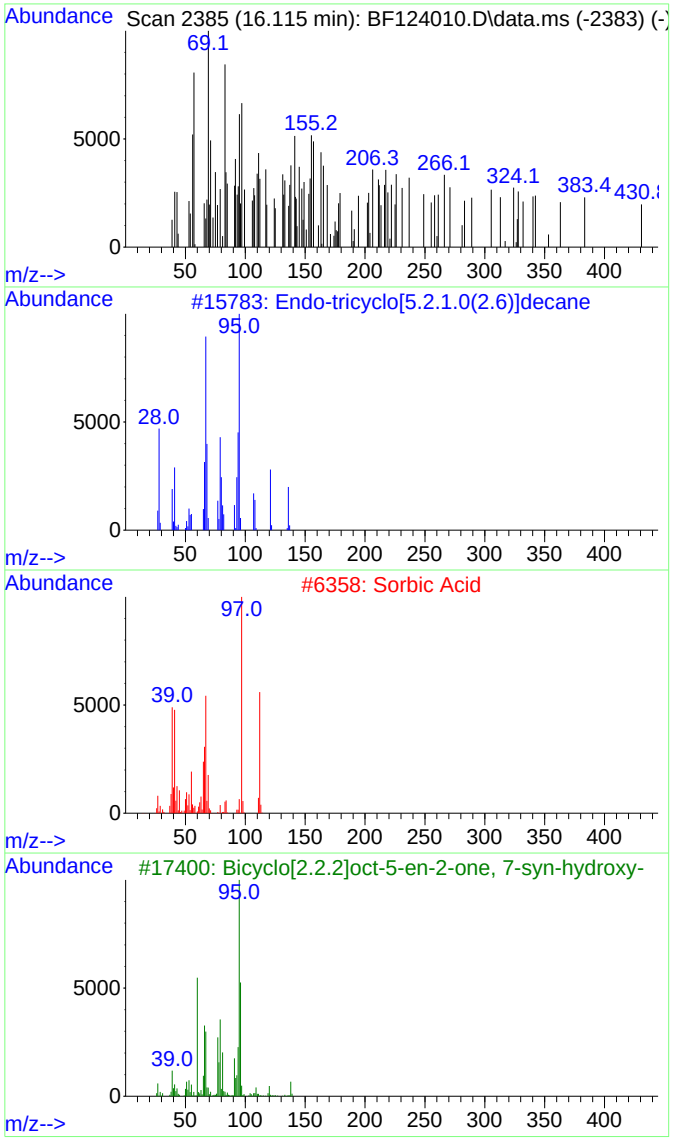
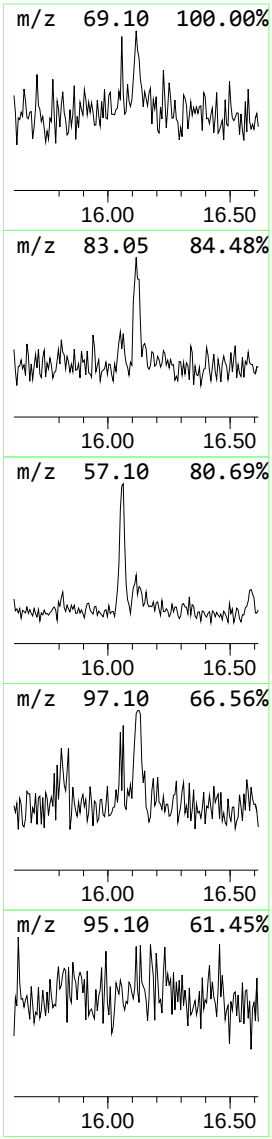
Peak Number 11 unknown16.11 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.115	4.50 ng	64685	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Endo-tricyclo[5.2.1.0(2.6)]decane	136	C10H16	1000215-28-8	18
2	Sorbic Acid	112	C6H8O2	000110-44-1	14
3	Bicyclo[2.2.2]oct-5-en-2-one, 7-...	138	C8H10O2	1000153-14-9	14
4	Spiro[bicyclo[3.3.0]octan-6-one-...	150	C10H14O	1000152-21-9	14
5	8-Thiabicyclo[5.1.0]octane	128	C7H12S	053907-79-2	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052021\
Data File : BF124010.D
Acq On : 20 May 2021 15:39
Operator : JU/CG
Sample : M2468-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-5-TP

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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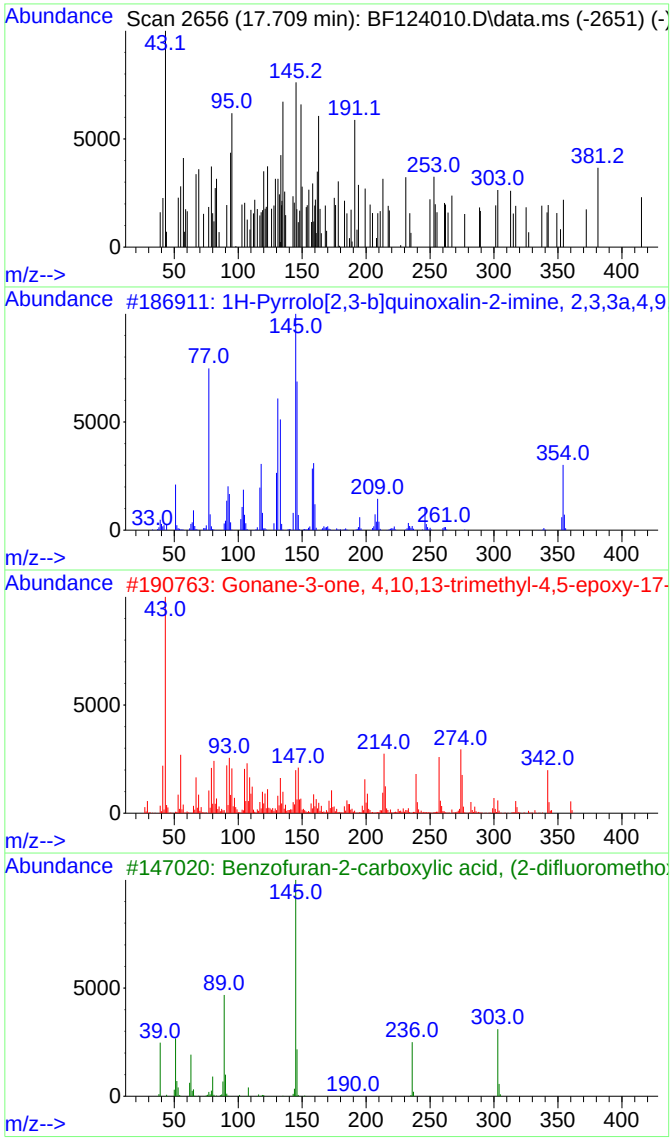
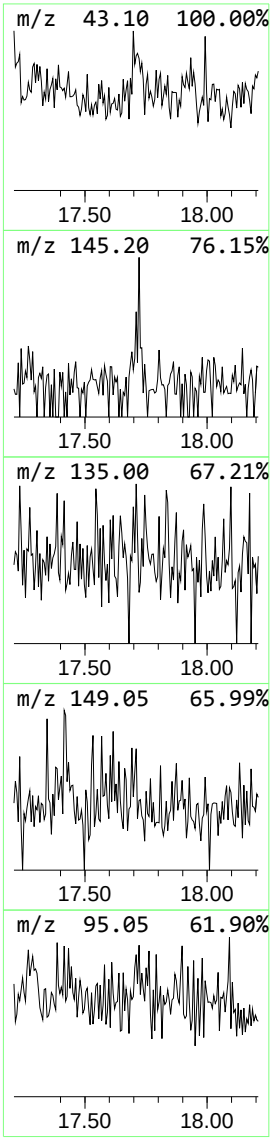
Peak Number 12 unknown17.70 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	4.99 ng	71713	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrrolo[2,3-b]quinoxalin-2-im...	354	C23H22N4	1000271-61-3	27
2	Gonane-3-one, 4,10,13-trimethyl-...	360	C22H32O4	1000198-01-3	17
3	Benzofuran-2-carboxylic acid, (2...	303	C16H11F2NO3	1000311-07-8	9
4	3-Amino-2-(3-chloro-phenoxymethy...	301	C15H12ClN3O2	1000294-99-0	9
5	N-(4-Methoxy-2-nitro-phenyl)-2-(...	372	C17H16N4O4S	1000295-76-2	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052021\
Data File : BF124010.D
Acq On : 20 May 2021 15:39
Operator : JU/CG
Sample : M2468-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-5-TP

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...	2.134	17.1	ng	293407	1	6.904	343537	20.0
2-Pentanone, 4-...	5.104	3.6	ng	61989	1	6.904	343537	20.0
Dodecanoic acid	11.951	2.4	ng	63084	4	11.433	527848	20.0
unknown13.85	13.851	11.2	ng	257197	5	14.074	460715	20.0
unknown13.91	13.916	7.3	ng	168003	5	14.074	460715	20.0
unknown14.55	14.557	3.5	ng	80701	5	14.074	460715	20.0
unknown15.12	15.127	2.3	ng	33711	6	15.574	287642	20.0
unknown15.21	15.210	2.7	ng	38712	6	15.574	287642	20.0
Eicosane, 2,6,1...	16.057	5.5	ng	78356	6	15.574	287642	20.0
unknown16.11	16.115	4.5	ng	64685	6	15.574	287642	20.0
unknown17.70	17.709	5.0	ng	71713	6	15.574	287642	20.0