LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RB-09-(2.8-3.6)

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126701.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.299	29	36	42	rVB	434234	555927	13.52%	1.752%
2	4.099	338	342	348	rVB	35356	43068	1.05%	0.136%
3	5.193	524	528	533	rVB	50332	59809	1.45%	0.189%
4	5.575	588	593	596	rBV	3561883	3357826	81.64%	10.583%
5	6.569	756	762	765	rBV	3919128	4017073	97.67%	12.661%
6	6.951	824	827	831	rBV	1215642	1098862	26.72%	3.463%
7	7.516	918	923	926	rBV	2808267	2561983	62.29%	8.075%
8	8.234	1041	1045	1049	rBV	1505336	1459523	35.49%	4.600%
9	9.316	1223	1229	1232	rBV	4323759	4112872	100.00%	12.963%
10	9.386	1237	1241	1243	rBV	68533	57190	1.39%	0.180%
11	9.998	1341	1345	1348	rBV	1911775	1619662	39.38%	5.105%
12	10.416	1408	1416	1419	rBV4	35948	50227	1.22%	0.158%
13	10.786	1474	1479	1482	rBV	2704199	2304375	56.03%	7.263%
14	10.904	1495	1499	1502	rVB2	31445	43912	1.07%	0.138%
15	11.375	1575	1579	1584	rVB6	29104	49481	1.20%	0.156%
16	11.486	1595	1598	1601	rBV	1883133	1611160	39.17%	5.078%
17	11.510	1601	1602	1606	rVV	287681	183492	4.46%	0.578%
18	11.563	1608	1611	1614	rVB	47048	43663	1.06%	0.138%
19	11.986	1680	1683	1686	rBV2	35869	50941	1.24%	0.161%
20	12.098	1700	1702	1705	rBV2	41136	43880	1.07%	0.138%
21	12.704	1802	1805	1808	rBV	391793	317020	7.71%	0.999%
22	12.933	1838	1844	1848	rBV	384937	354311	8.61%	1.117%
23	13.080	1864	1869	1872	rVB	3714683	3307353	80.41%	10.424%
24	13.145	1877	1880	1885	rBV4	24409	42101	1.02%	0.133%
25	13.363	1914	1917	1921	rVB3	42559	45196	1.10%	0.142%
26	13.980	2018	2022	2033	rVB4	120916	236049	5.74%	0.744%
27	14.133	2043	2048	2051	rBV	1054215	1078013	26.21%	3.398%
28	14.163	2051	2053	2059	rVB	162561	150250	3.65%	0.474%
29	14.239	2061	2066	2070	rBV5	26791	46115	1.12%	0.145%
30	14.280	2070	2073	2077	rBV2	36229	49855	1.21%	0.157%
31	14.521	2110	2114	2117	rVB	68830	60783	1.48%	0.192%
32	14.821	2162	2165	2169	rBV	66682	67821	1.65%	0.214%
33	14.904	2175	2179	2186	rBV3	100474	147805	3.59%	0.466%
34	14.992	2191	2194	2199	rVB2	127488	135268	3.29%	0.426%
35	15.174	2222	2225	2226	rBV	59350	60346	1.47%	0.190%
36	15.204	2226	2230	2233	rVV	112169	157110	3.82%	0.495%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.321	2246	2250	2254	rVB3	47642	63522	1.54%	0.200%
38	15.521	2279	2284	2289	rBV	90607	114907	2.79%	0.362%
39	15.586	2291	2295	2302	rVB	98040	121669	2.96%	0.383%
40	15.657	2302	2307	2325	rBV	630321	879117	21.37%	2.771%
41	15.886	2341	2346	2353	rVB	86906	134859	3.28%	0.425%
42	16.068	2373	2377	2382	rVB3	34770	47136	1.15%	0.149%
43	16.145	2384	2390	2396	rVB6	24879	54895	1.33%	0.173%
44	16.327	2417	2421	2430	rVB3	41337	74655	1.82%	0.235%
45	16.498	2445	2450	2456	rBV2	31418	60614	1.47%	0.191%
46	16.792	2495	2500	2509	rBV2	56953	115614	2.81%	0.364%
47	17.039	2532	2542	2548	rVB6	29103	74102	1.80%	0.234%
48	17.198	2564	2569	2578	rVB2	47225	102653	2.50%	0.324%
49	17.380	2595	2600	2608	rVB6	38660	89918	2.19%	0.283%
50	17.468	2608	2615	2626	rBV8	21916	68057	1.65%	0.215%
51	17.592	2631	2636	2642	rVB9	31023	60624	1.47%	0.191%
52	17.674	2644	2650	2656	rVB	41925	85498	2.08%	0.269%

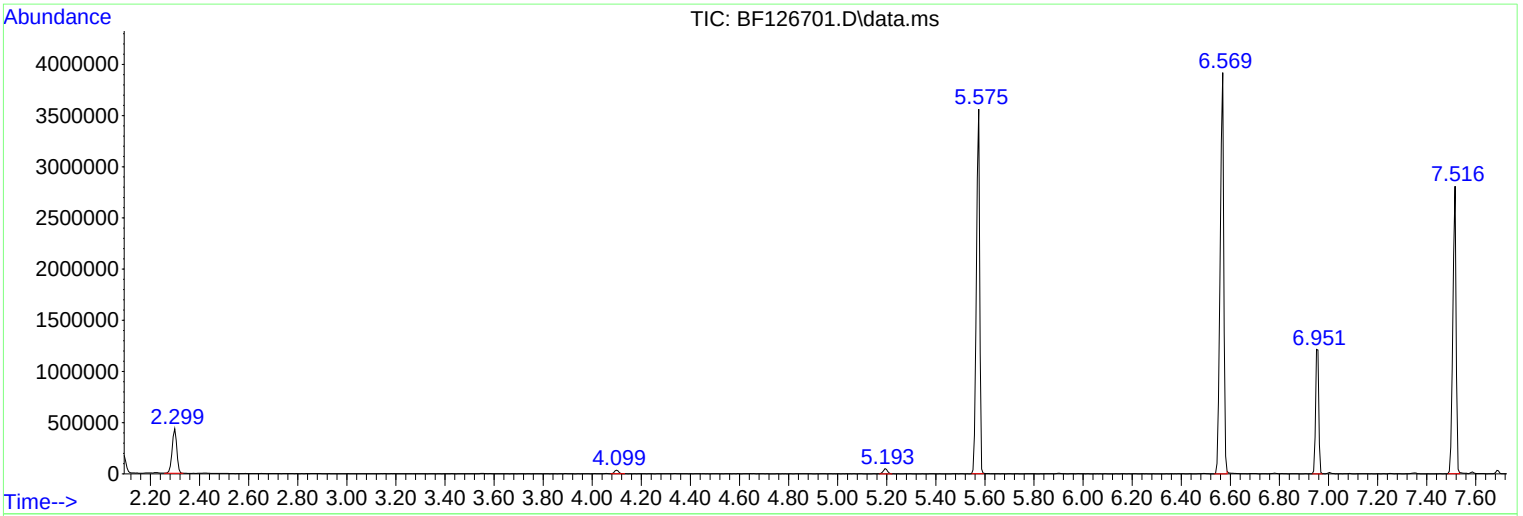
Sum of corrected areas: 31728162

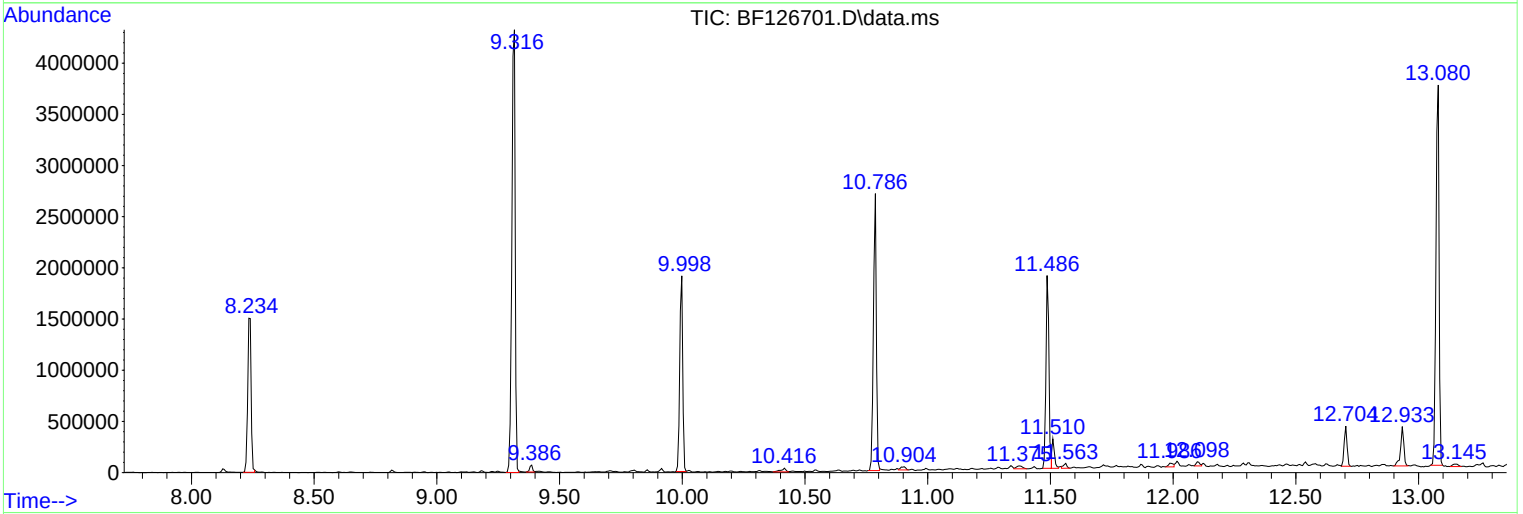
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

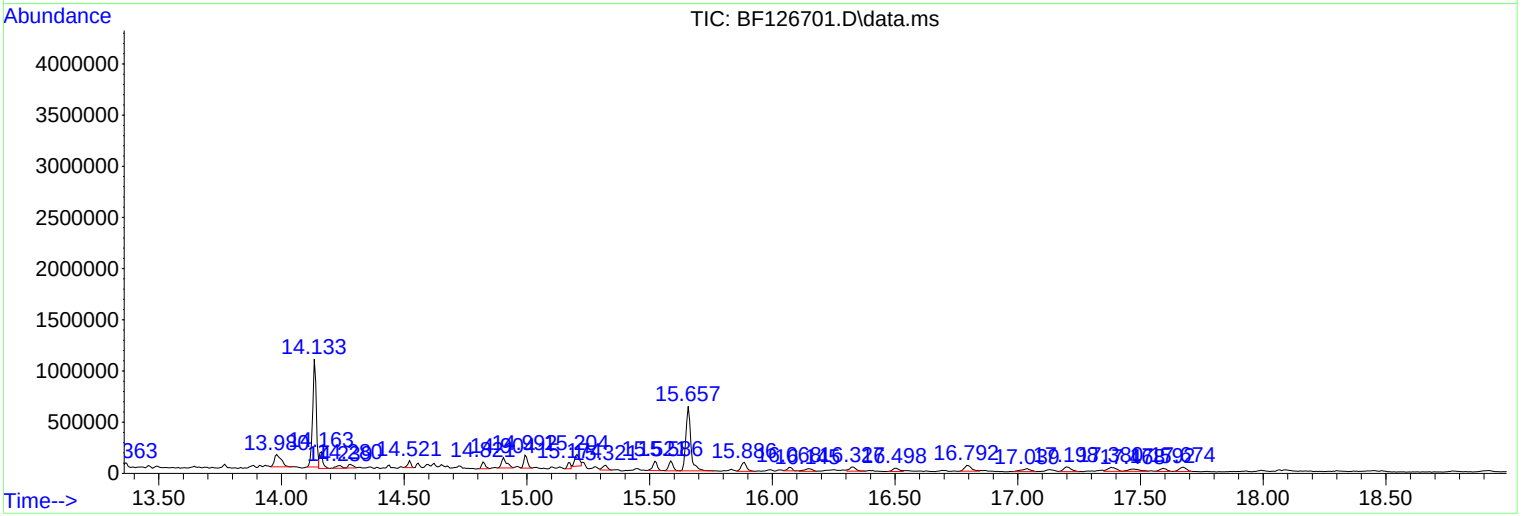
Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

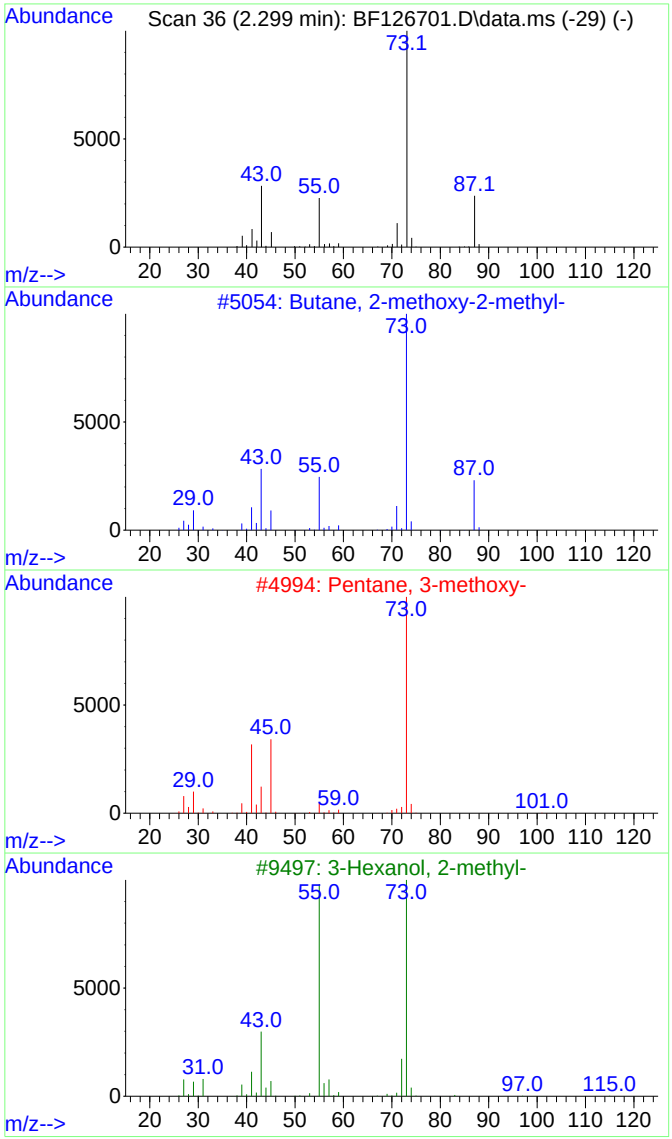
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

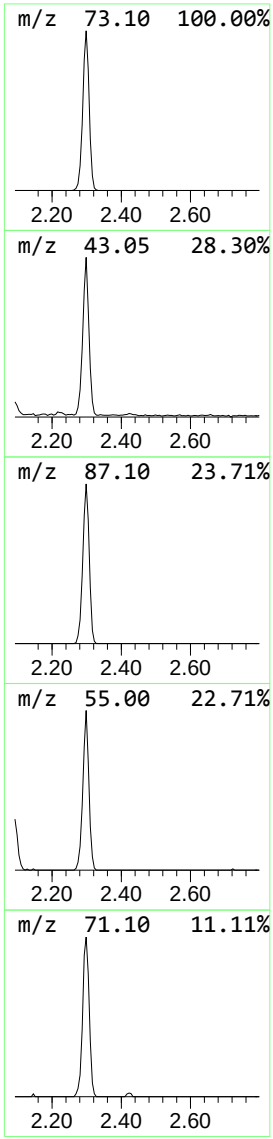
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	10.12 ng	555927	1,4-Dichlorobenzene-d4	6.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

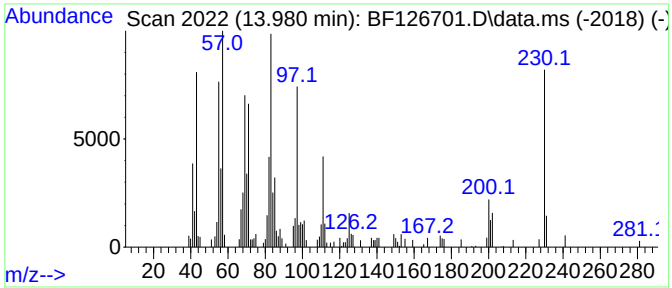
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

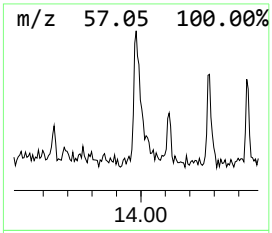
****

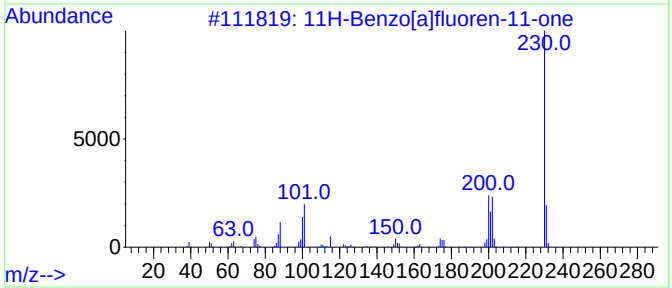
Peak Number 2 11H-Benzo[a]fluoren-11-one Concentration Rank 2

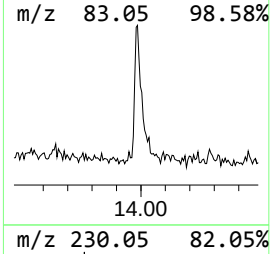
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	4.38 ng	236049	Chrysene-d12	14.133

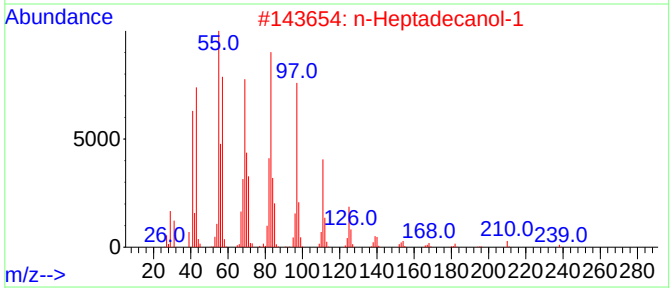
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	90
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	64
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	62
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	58
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	58

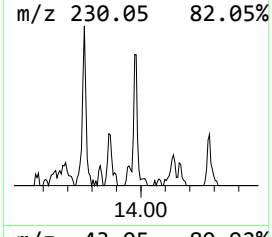


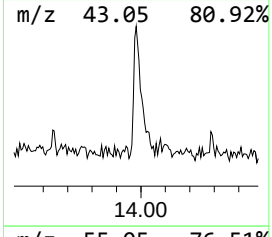


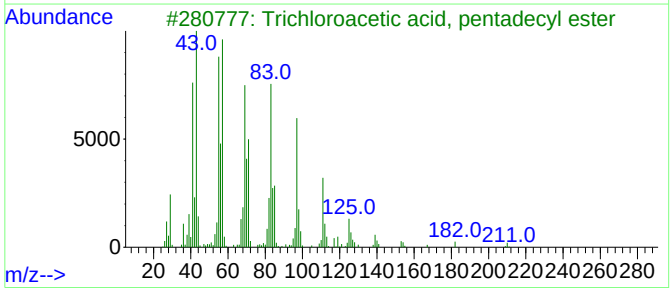


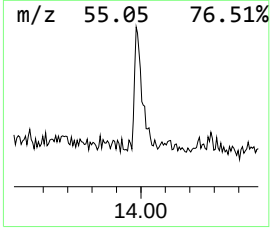












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

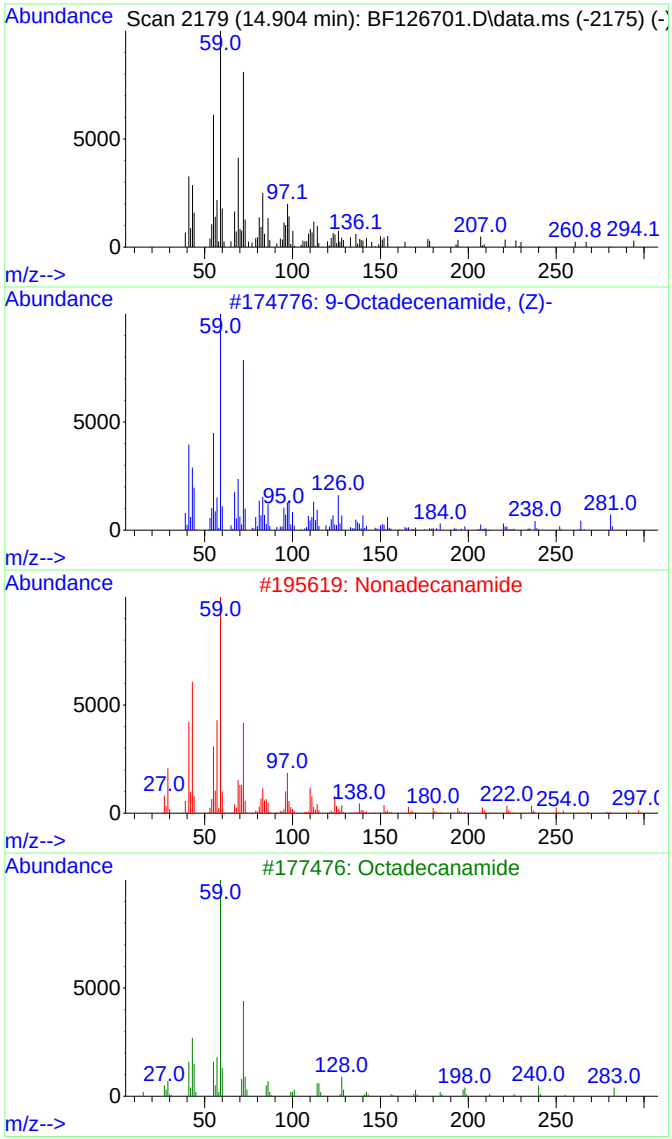
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

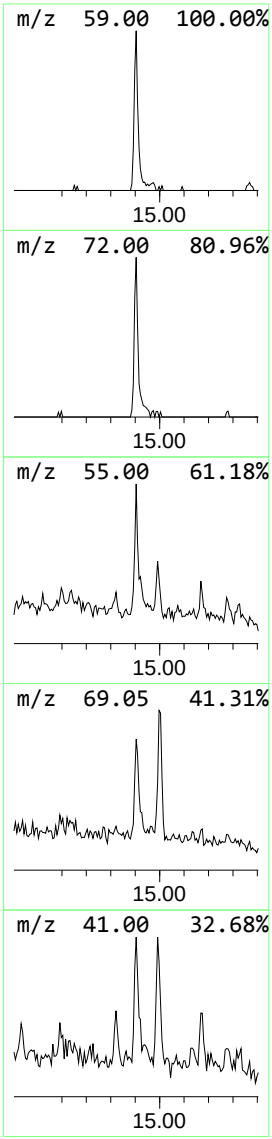
****

Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	3.36 ng	147805	Perylene-d12	15.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2	Nonadecanamide	297	C19H39NO	058185-32-3	38
3	Octadecanamide	283	C18H37NO	000124-26-5	38
4	Succinic acid, dodec-2-en-1-yl 2...	342	C19H34O5	1000390-75-0	35
5	Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

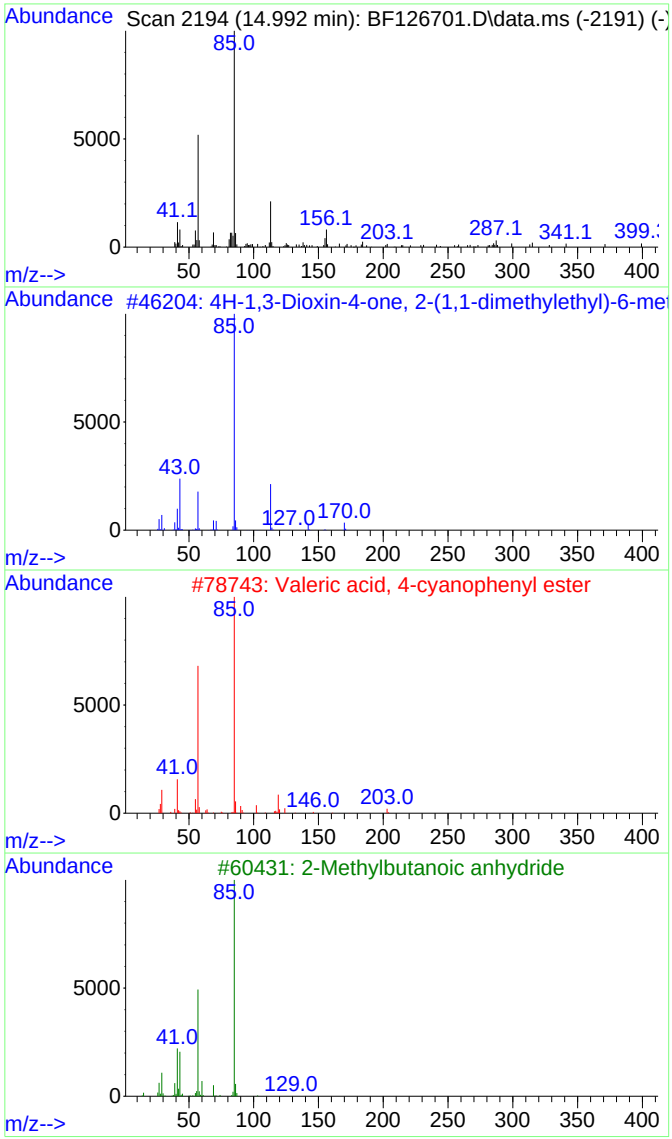
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

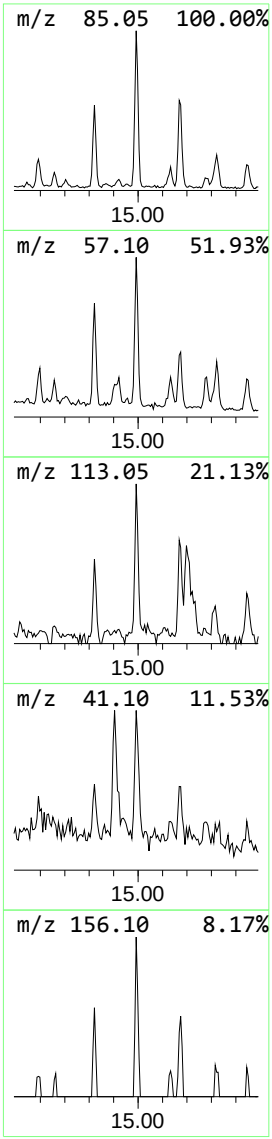
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-1,3-Dioxin-4-one, 2-(1,1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	3.08 ng	135268	Perylene-d12	15.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,3-Dioxin-4-one, 2-(1,1-dime...	170	C9H14O3	107289-20-3	64
2	Valeric acid, 4-cyanophenyl ester	203	C12H13NO2	1000307-98-7	50
3	2-Methylbutanoic anhydride	186	C10H18O3	001468-39-9	50
4	Valeric acid, 2,5-dichlorophenyl...	246	C11H12Cl2O2	1000325-72-5	50
5	Valeric anhydride	186	C10H18O3	002082-59-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

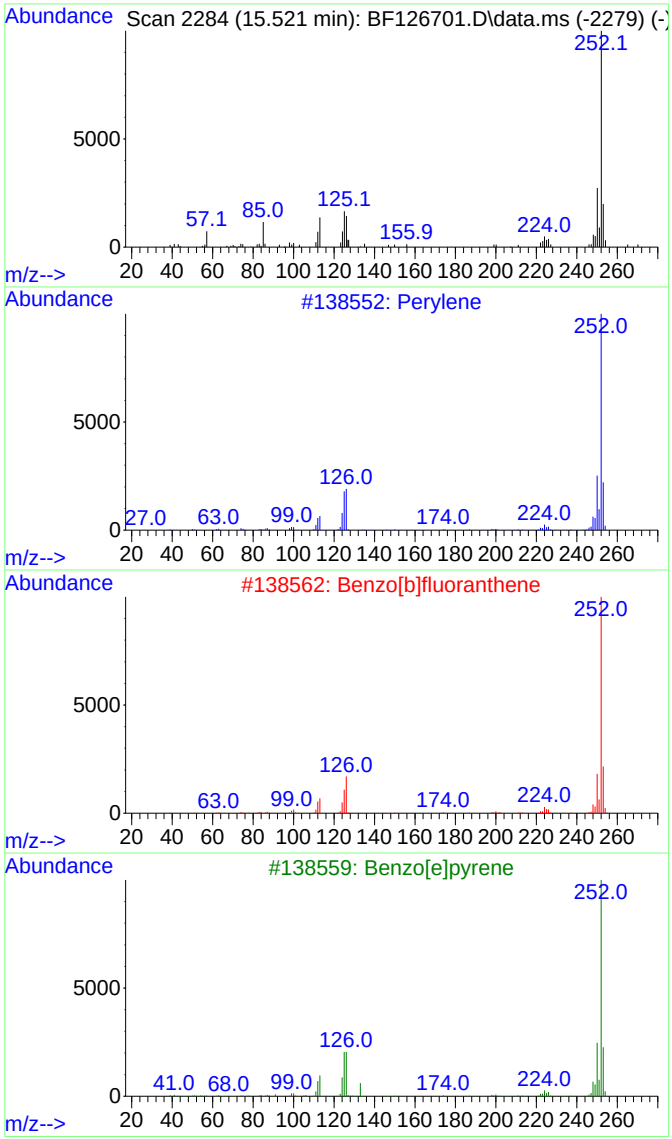
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

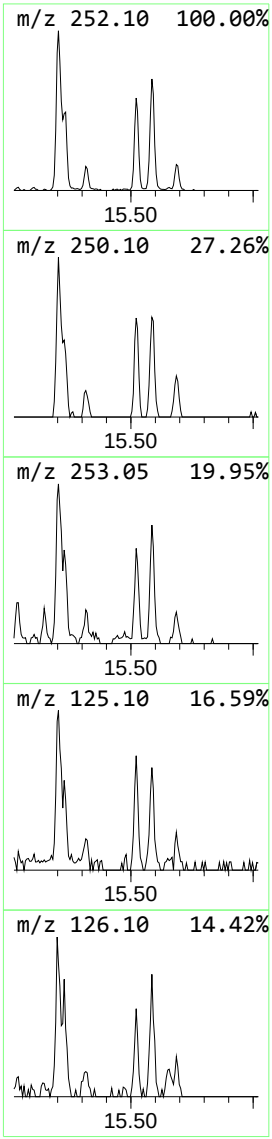
****

Peak Number 5 Perylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.521	2.61 ng	114907	Perylene-d12	15.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	96
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
3	Benzo[e]pyrene	252	C20H12	000192-97-2	95
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

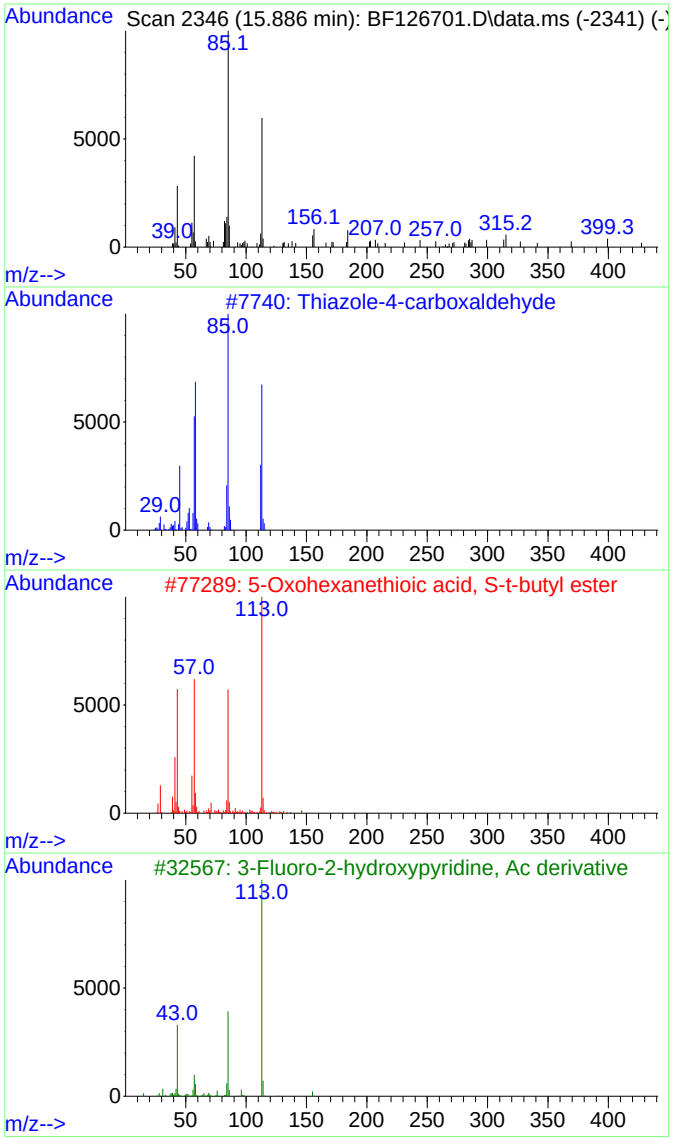
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

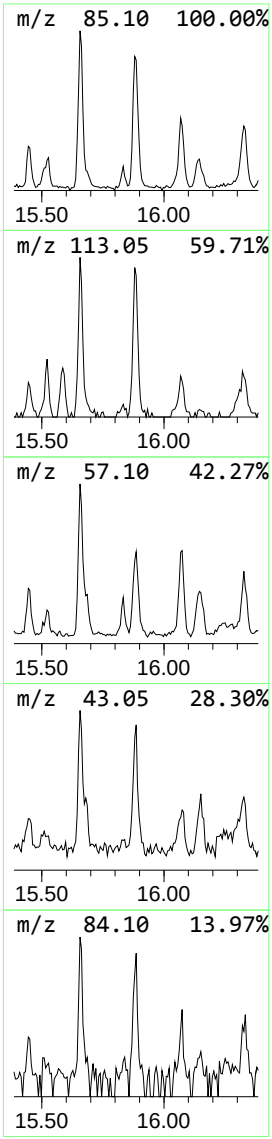
****

Peak Number 6 Thiazole-4-carboxaldehyde Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	3.07 ng	134859	Perylene-d12	15.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazole-4-carboxaldehyde	113	C4H3NOS	003364-80-5	80
2	5-Oxohexanethioic acid, S-t-buty...	202	C10H18O2S	1000194-60-8	72
3	3-Fluoro-2-hydroxypyridine, Ac d...	155	C7H6FNO2	1000496-78-8	56
4	Malonic acid, di(2-methylpent-3-...	272	C15H28O4	1000349-05-7	47
5	3-Methylpentan-3-yl 2-methylbuta...	186	C11H22O2	1000372-73-3	47





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Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

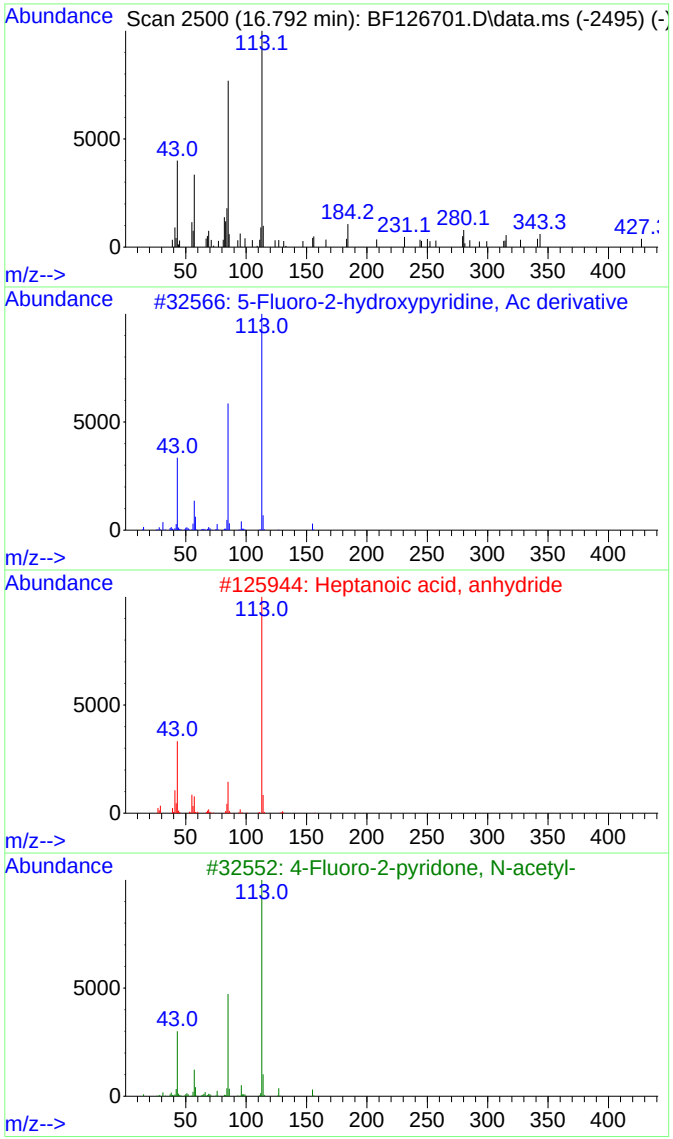
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

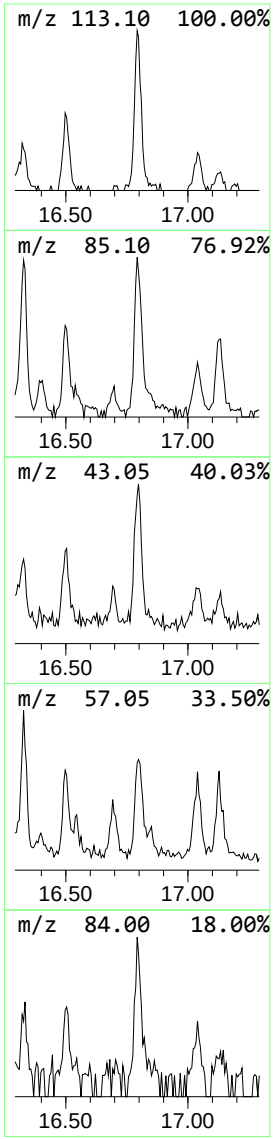
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 5-Fluoro-2-hydroxypyridine,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.792	2.63 ng	115614	Perylene-d12	15.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-hydroxypyridine, Ac d...	155	C7H6FNO2	1000496-67-3	64
2	Heptanoic acid, anhydride	242	C14H26O3	000626-27-7	64
3	4-Fluoro-2-pyridone, N-acetyl-	155	C7H6FNO2	1000508-33-5	47
4	Heptanoic acid, 3-nitrophenyl ester	251	C13H17NO4	056052-18-7	38
5	4-Methylamino-2(5H)-furanone	113	C5H7NO2	1000427-45-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

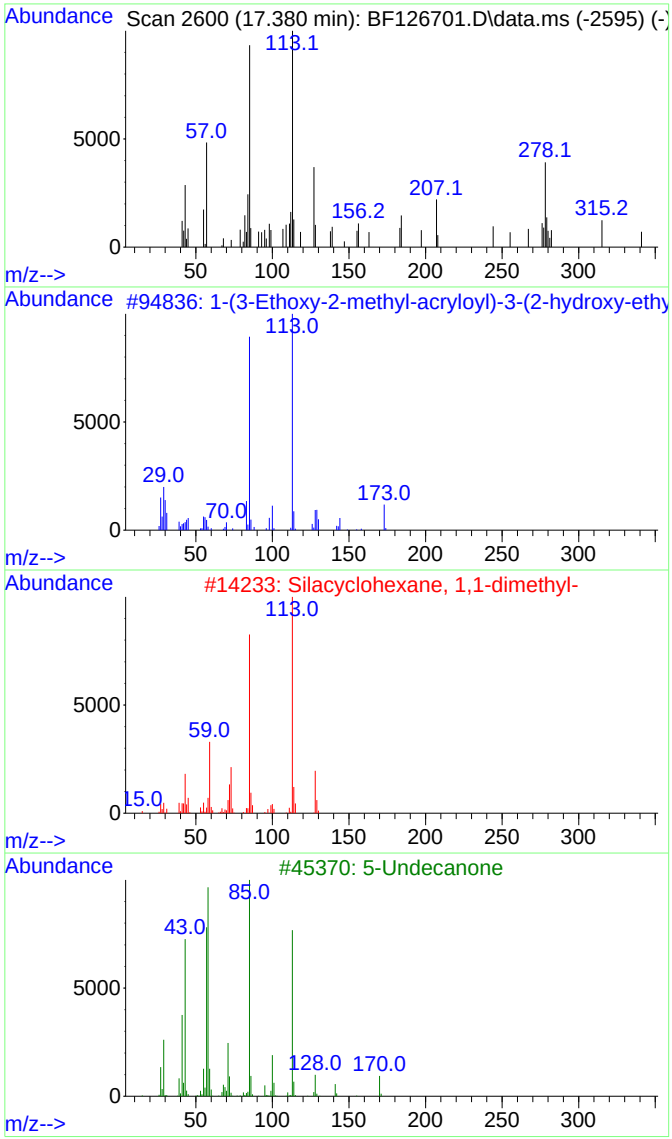
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

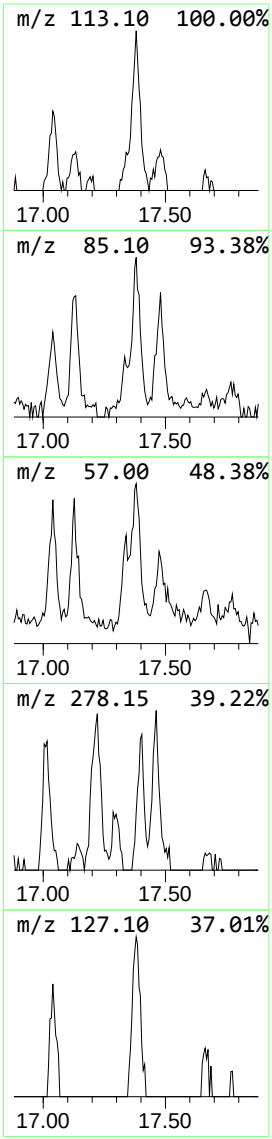
****

Peak Number 8 unknown17.380 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.380	2.05 ng	89918	Perylene-d12	15.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(3-Ethoxy-2-methyl-acryloyl)-3...	216	C9H16N2O4	1000188-24-4	43
2	Silacyclohexane, 1,1-dimethyl-	128	C7H16Si	004040-74-8	43
3	5-Undecanone	170	C11H22O	033083-83-9	37
4	2-Propyn-1-ol, 3-(trimethylsilyl)-	128	C6H12OSi	005272-36-6	37
5	2,2-Dimethyl-propionic acid, 2-(...	260	C13H24O5	128435-09-6	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012622\
Data File : BF126701.D
Acq On : 26 Jan 2022 21:51
Operator : CG/JU
Sample : N1266-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-09-(2.8-3.6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.299	10.1	ng	555927	1	6.957	1098860	20.0
11H-Benzo[a]flu...	13.980	4.4	ng	236049	5	14.133	1078010	20.0
9-Octadecenamid...	14.904	3.4	ng	147805	6	15.657	879117	20.0
4H-1,3-Dioxin-4...	14.992	3.1	ng	135268	6	15.657	879117	20.0
Perylene	15.521	2.6	ng	114907	6	15.657	879117	20.0
Thiazole-4-carb...	15.886	3.1	ng	134859	6	15.657	879117	20.0
5-Fluoro-2-hydr...	16.792	2.6	ng	115614	6	15.657	879117	20.0
unknown17.380	17.380	2.0	ng	89918	6	15.657	879117	20.0