LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082520\
Data File : BF121431.D
Acq On : 25 Aug 2020 17:03
Operator : JU/CG
Sample : L3784-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-11

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-BF081920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	473	476	485	rBV	33586	48897	1.45%	0.180%
2	5.310	544	548	572	rBV	2038483	2351641	69.91%	8.670%
3	6.346	719	724	741	rBV	2190232	2377440	70.68%	8.766%
4	6.693	780	783	793	rVB	1002050	802190	23.85%	2.958%
5	7.263	875	880	892	rBV	1791544	1660128	49.35%	6.121%
6	7.975	998	1001	1018	rBV	1147359	1119123	33.27%	4.126%
7	9.051	1180	1184	1195	rBV	3117688	2977148	88.51%	10.977%
8	9.445	1248	1251	1260	rVB	262830	248603	7.39%	0.917%
9	9.728	1295	1299	1309	rVB	1533081	1315205	39.10%	4.849%
10	10.522	1429	1434	1445	rBV	1864951	1912251	56.85%	7.050%
11	10.645	1450	1455	1463	rVB3	24045	37188	1.11%	0.137%
12	11.210	1547	1551	1554	rBV	1543251	1434594	42.65%	5.289%
13	11.233	1554	1555	1559	rVB	168230	113788	3.38%	0.420%
14	11.451	1585	1592	1597	rBV3	20645	37344	1.11%	0.138%
15	11.745	1639	1642	1645	rBV2	73581	70259	2.09%	0.259%
16	11.822	1652	1655	1658	rBV	38059	37992	1.13%	0.140%
17	12.422	1753	1757	1762	rVB	385271	324083	9.63%	1.195%
18	12.651	1789	1796	1799	rBV	338074	347175	10.32%	1.280%
19	12.798	1814	1821	1825	rBV	3045706	3363663	100.00%	12.402%
20	12.869	1829	1833	1838	rBV4	28048	42206	1.25%	0.156%
21	12.980	1849	1852	1855	rVB2	45473	52032	1.55%	0.192%
22	13.027	1855	1860	1862	rBV3	40124	50569	1.50%	0.186%
23	13.080	1866	1869	1877	rVB3	46629	68382	2.03%	0.252%
24	13.369	1913	1918	1921	rBV3	39300	56855	1.69%	0.210%
25	13.492	1935	1939	1943	rVB	48836	55262	1.64%	0.204%
26	13.598	1951	1957	1959	rBV	50024	61708	1.83%	0.228%
27	13.704	1971	1975	1991	rVB2	371569	715039	21.26%	2.636%
28	13.851	1992	2000	2003	rBV	1600054	1731999	51.49%	6.386%
29	13.874	2003	2004	2011	rVB	232547	155521	4.62%	0.573%
30	14.016	2023	2028	2031	rBV3	60818	77785	2.31%	0.287%
31	14.239	2063	2066	2068	rVB	47825	43456	1.29%	0.160%
32	14.321	2075	2080	2082	rBV2	78391	97525	2.90%	0.360%
33	14.357	2082	2086	2093	rVB5	78170	163329	4.86%	0.602%
34	14.616	2127	2130	2133	rVB	77645	70640	2.10%	0.260%

LSC Area Percent Report

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Operator : JU/CG
Sample : L3784-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-11

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-BF081920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.863	2168	2172	2179	rBV	221051	397098	11.81%	1.464%
36	14.933	2180	2184	2187	rVB2	103277	117313	3.49%	0.433%
37	14.968	2187	2190	2194	rBV	46169	73808	2.19%	0.272%
38	15.145	2217	2220	2226	rVB	128880	154656	4.60%	0.570%
39	15.204	2226	2230	2235	rVB	163245	184664	5.49%	0.681%
40	15.263	2235	2240	2253	rBV	970271	1369214	40.71%	5.048%
41	15.680	2306	2311	2316	rBV	109068	155640	4.63%	0.574%
42	15.780	2320	2328	2333	rBV8	46868	149877	4.46%	0.553%
43	16.145	2386	2390	2393	rBV	33101	44763	1.33%	0.165%
44	16.627	2467	2472	2477	rBV2	75434	140638	4.18%	0.519%
45	16.686	2478	2482	2489	rVB2	46801	88280	2.62%	0.325%
46	17.039	2537	2542	2554	rVB	61861	131375	3.91%	0.484%
47	17.168	2558	2564	2575	rVB	28647	94193	2.80%	0.347%

Sum of corrected areas: 27122539

LSC Report - Integrated Chromatogram

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Data File : BF121431.D
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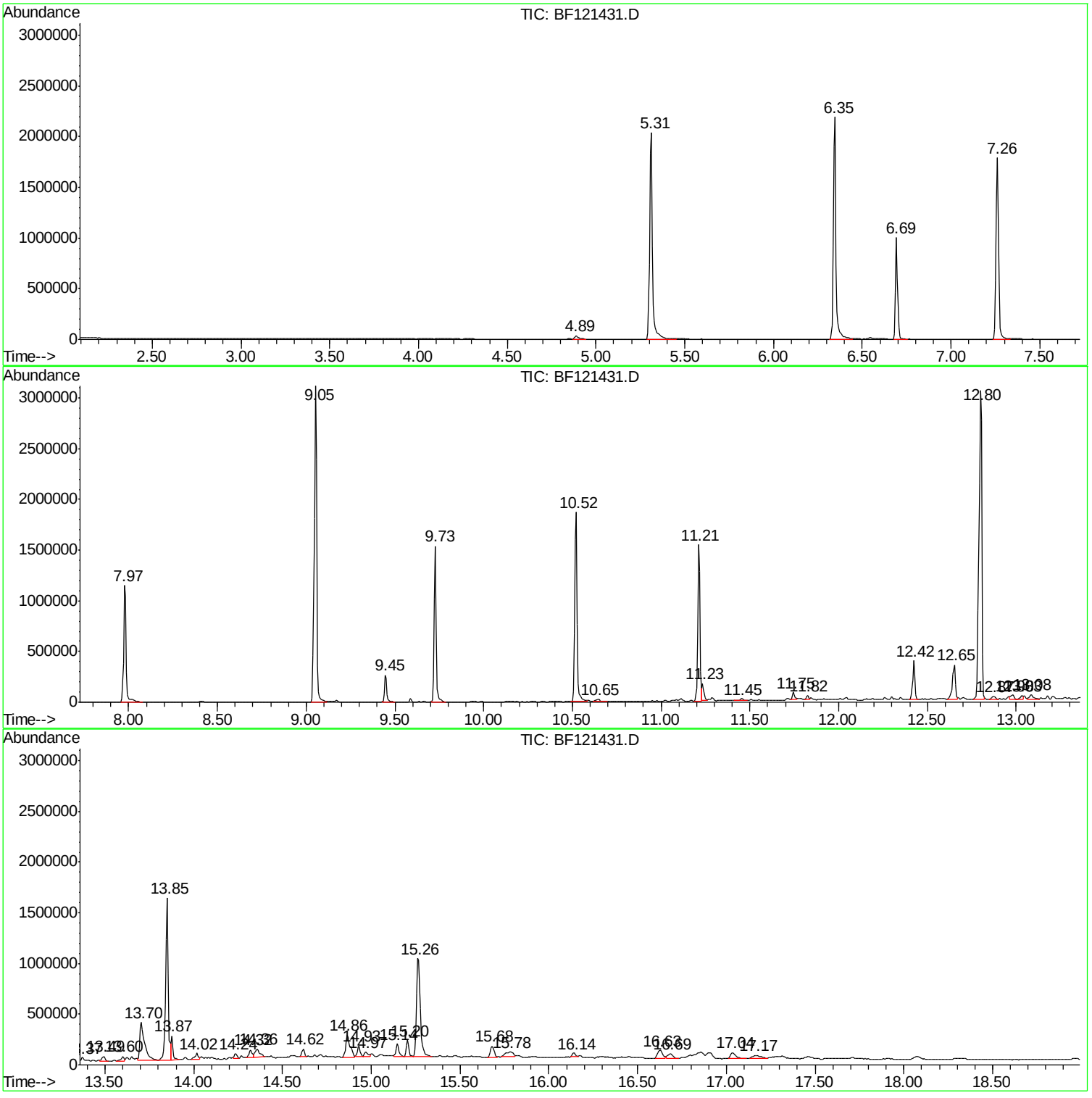
Sample : L3784-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082520\
Data File : BF121431.D
Acq On : 25 Aug 2020 17:03
Operator : JU/CG
Sample : L3784-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.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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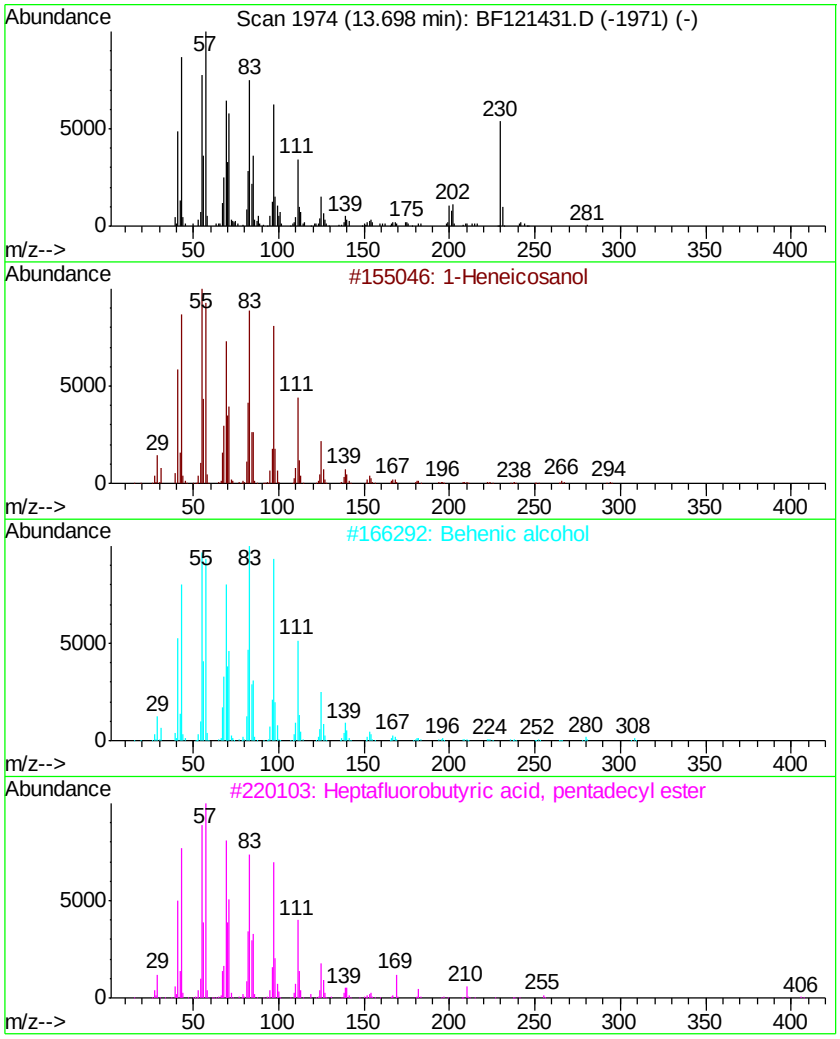
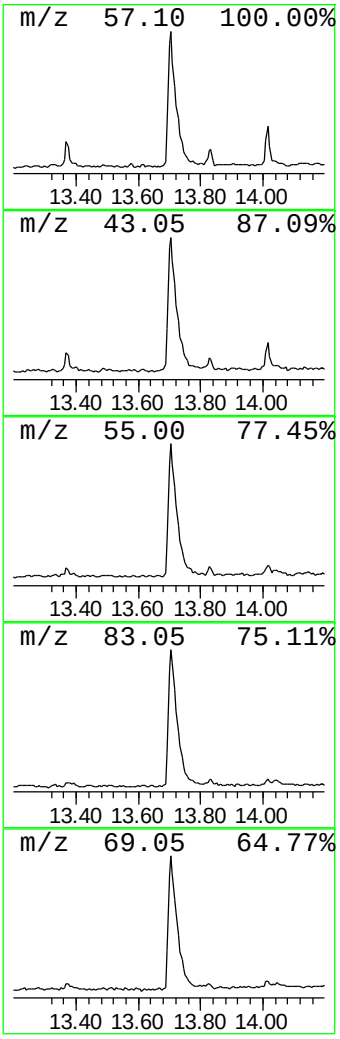
Peak Number 1 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	8.26 ng	715039	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082520\
Data File : BF121431.D
Acq On : 25 Aug 2020 17:03
Operator : JU/CG
Sample : L3784-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.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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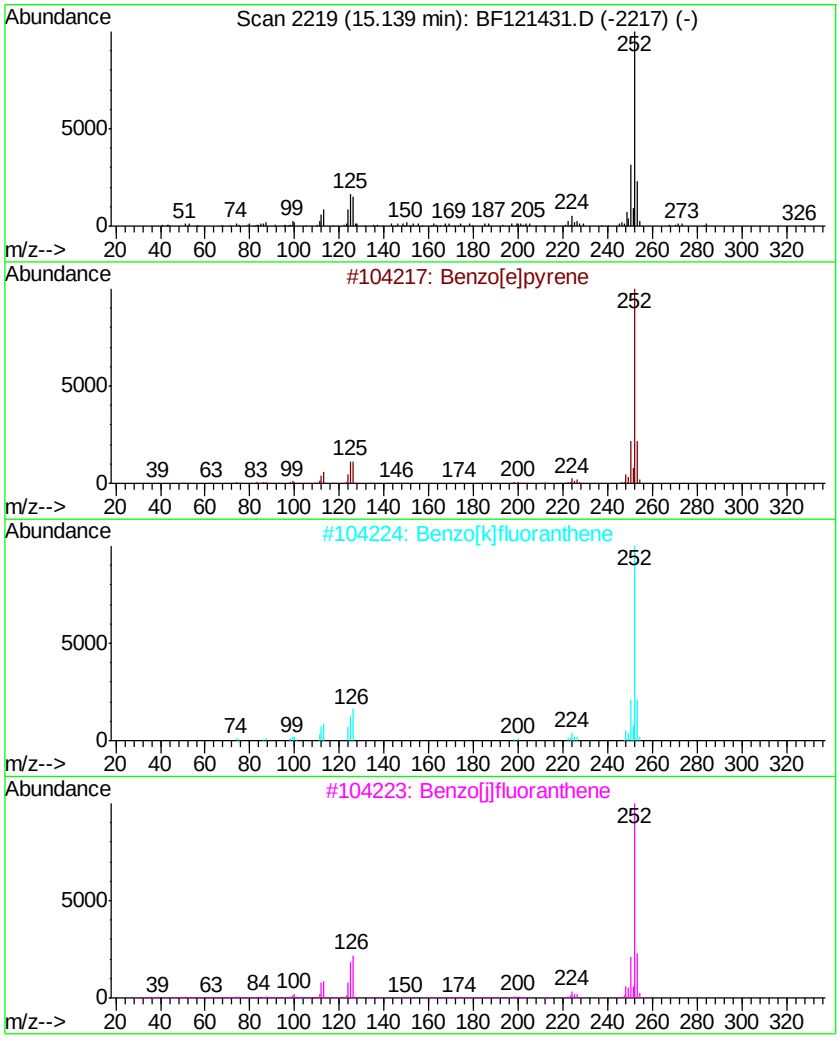
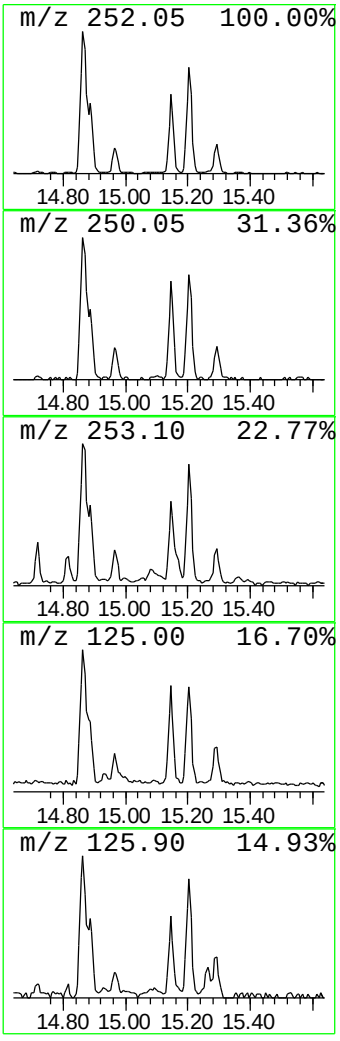
Peak Number 2 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	2.26 ng	154656	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
5	Perylene	252	C20H12	000198-55-0	95





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082520\
Data File : BF121431.D
Acq On : 25 Aug 2020 17:03
Operator : JU/CG
Sample : L3784-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.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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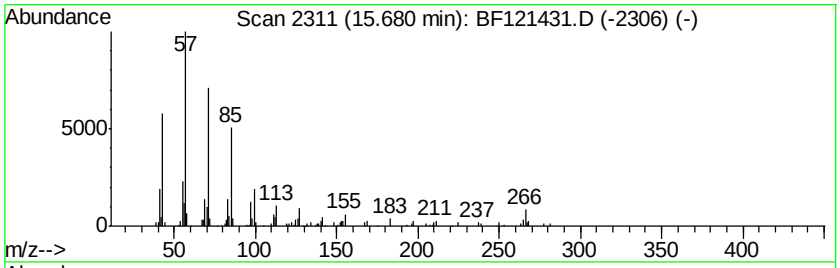
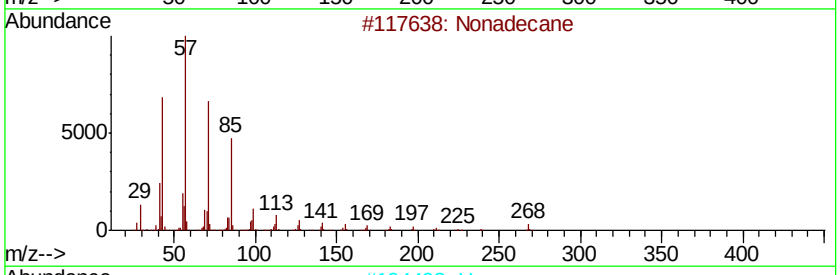
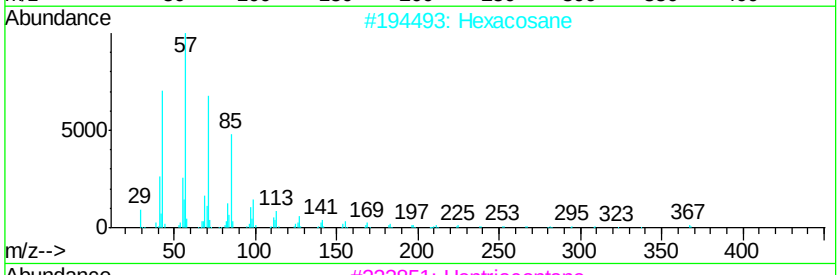
Peak Number 3 Nonadecane Concentration Rank 2

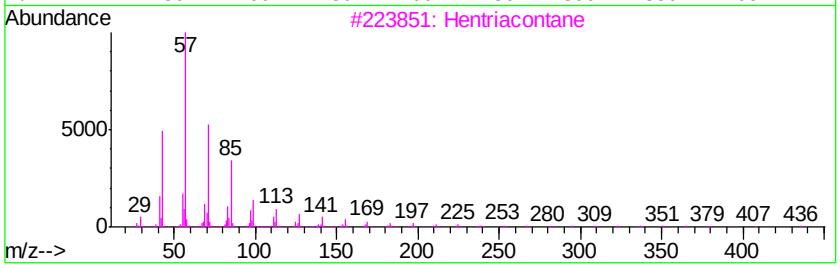
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	2.27 ng	155640	Perylene-d12	15.26

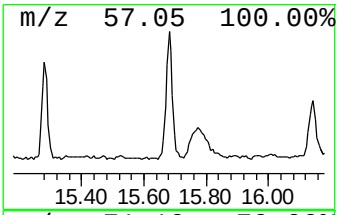
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Hexacosane	366	C26H54	000630-01-3	90
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	Heneicosane	296	C21H44	000629-94-7	90

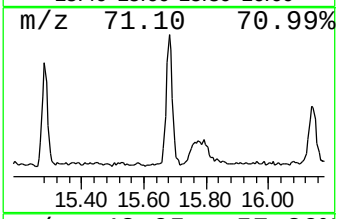


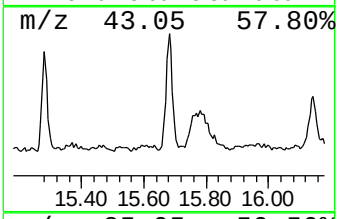


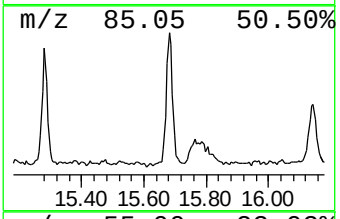


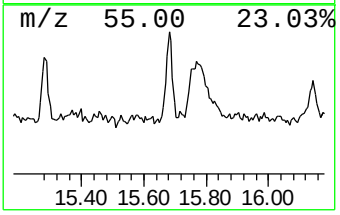












Library Search Compound Report

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Data File : BF121431.D
Acq On : 25 Aug 2020 17:03
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Sample : L3784-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

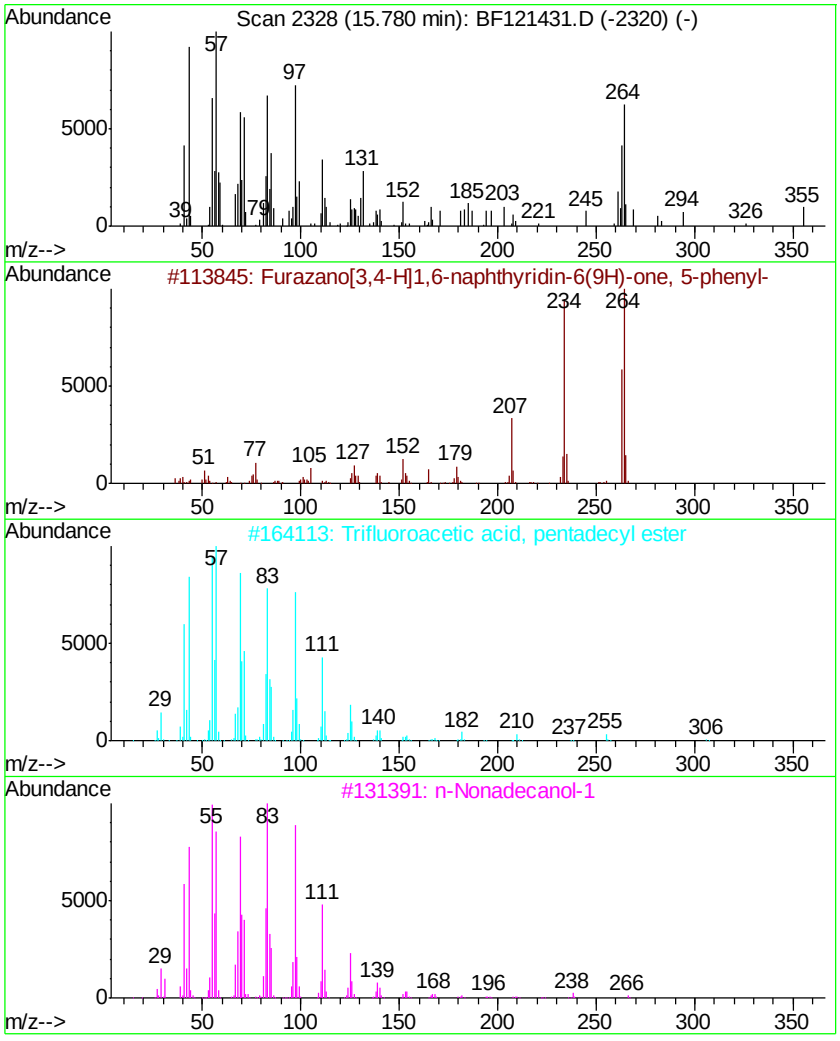
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

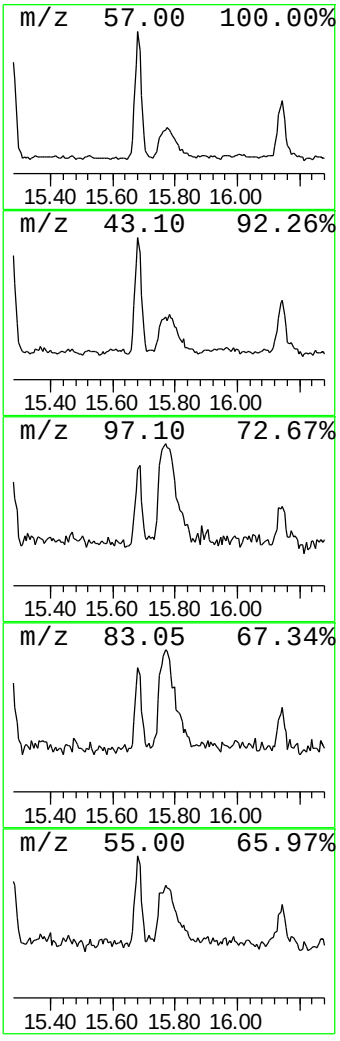
****

Peak Number 4 unknown15.78 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	2.19 ng	149877	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furazano[3,4-H]1,6-naphthyridin-...	264	C14H8N4O2	296245-19-7	30
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	25
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	25
4	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	20
5	1-Hentetracontanol	593	C41H84O	040710-42-7	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082520\
Data File : BF121431.D
Acq On : 25 Aug 2020 17:03
Operator : JU/CG
Sample : L3784-04
Misc :
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ClientSampleId : RO-11

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.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
1-Heneicosanol	13.70	8.3	ng	715039	5	13.85	1732000	20.0
Benzo[e]pyrene	15.14	2.3	ng	154656	6	15.26	1369210	20.0
Nonadecane	15.68	2.3	ng	155640	6	15.26	1369210	20.0
unknown15.78	15.78	2.2	ng	149877	6	15.26	1369210	20.0