LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100220\
Data File : BF121793.D
Acq On : 2 Oct 2020 14:38
Operator : JU/CG
Sample : L4198-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-10

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-BF091020.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	4.987	489	493	504	rVB	50404	66925	1.86%	0.229%
2	5.387	557	561	578	rBV	2943004	2920419	81.30%	10.005%
3	6.404	729	734	747	rBV	2908572	3018678	84.03%	10.341%
4	6.592	763	766	780	rBV	87141	114587	3.19%	0.393%
5	6.763	791	795	798	rBV	951834	796757	22.18%	2.729%
6	7.328	885	891	894	rBV	2113031	2088785	58.15%	7.156%
7	8.045	1008	1013	1016	rBV	1161425	1061167	29.54%	3.635%
8	9.122	1190	1196	1199	rBV	3755322	3592358	100.00%	12.306%
9	9.516	1259	1263	1266	rBV	405510	335805	9.35%	1.150%
10	9.798	1305	1311	1314	rBV	1389771	1202249	33.47%	4.119%
11	10.586	1440	1445	1449	rBV	2268961	2126199	59.19%	7.284%
12	10.716	1461	1467	1469	rBV5	28924	40390	1.12%	0.138%
13	11.280	1558	1563	1565	rBV	1400187	1165718	32.45%	3.993%
14	11.304	1565	1567	1570	rVV	309540	247095	6.88%	0.846%
15	11.357	1574	1576	1579	rVB	68456	51938	1.45%	0.178%
16	11.516	1596	1603	1609	rBV2	31225	58471	1.63%	0.200%
17	11.780	1645	1648	1650	rBV	56284	46692	1.30%	0.160%
18	11.810	1650	1653	1657	rVV	107581	88291	2.46%	0.302%
19	11.892	1664	1667	1669	rBV	90358	88426	2.46%	0.303%
20	11.916	1669	1671	1676	rVB	47399	41632	1.16%	0.143%
21	12.333	1739	1742	1744	rBV	50741	51789	1.44%	0.177%
22	12.416	1753	1756	1764	rBV2	50375	58346	1.62%	0.200%
23	12.492	1764	1769	1774	rVB	554151	471996	13.14%	1.617%
24	12.721	1802	1808	1810	rBV	476581	483735	13.47%	1.657%
25	12.768	1814	1816	1821	rVB4	45791	55188	1.54%	0.189%
26	12.868	1824	1833	1836	rBV	3548806	3242474	90.26%	11.108%
27	12.939	1840	1845	1849	rBV2	47682	77386	2.15%	0.265%
28	13.027	1857	1860	1862	rBV3	41212	57567	1.60%	0.197%
29	13.051	1862	1864	1867	rVB	68391	56724	1.58%	0.194%
30	13.098	1867	1872	1873	rBV2	59589	72634	2.02%	0.249%
31	13.151	1877	1881	1884	rBV	66018	72593	2.02%	0.249%
32	13.274	1899	1902	1906	rBV	42151	37804	1.05%	0.130%
33	13.439	1925	1930	1933	rBV2	71879	84586	2.35%	0.290%
34	13.557	1944	1950	1954	rBV	76061	94149	2.62%	0.323%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : RO-10

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-BF091020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.662	1964	1968	1971	rBV2	55863	79842	2.22%	0.274%
36	13.721	1975	1978	1982	rVV3	47881	68979	1.92%	0.236%
37	13.768	1982	1986	1995	rVB2	491711	636938	17.73%	2.182%
38	13.915	2003	2011	2014	rBV2	982856	1266766	35.26%	4.340%
39	13.939	2014	2015	2022	rVB	227927	212268	5.91%	0.727%
40	14.021	2024	2029	2031	rBV2	32968	40891	1.14%	0.140%
41	14.086	2036	2040	2043	rBV2	95226	103884	2.89%	0.356%
42	14.304	2075	2077	2080	rVB	58330	43639	1.21%	0.149%
43	14.386	2087	2091	2093	rBV	111299	123396	3.43%	0.423%
44	14.509	2108	2112	2115	rBV2	31529	40733	1.13%	0.140%
45	14.686	2136	2142	2145	rBV2	85463	109582	3.05%	0.375%
46	14.757	2151	2154	2157	rBV	52286	54020	1.50%	0.185%
47	14.939	2181	2185	2188	rBV	222185	304971	8.49%	1.045%
48	15.009	2194	2197	2200	rVB	88523	85790	2.39%	0.294%
49	15.045	2200	2203	2207	rBV2	48796	58644	1.63%	0.201%
50	15.233	2231	2235	2241	rVB	123972	153828	4.28%	0.527%
51	15.292	2241	2245	2249	rVV	170430	193551	5.39%	0.663%
52	15.357	2251	2256	2268	rVB	636435	922808	25.69%	3.161%
53	15.792	2326	2330	2336	rVB	73246	103879	2.89%	0.356%
54	15.862	2338	2342	2352	rVB7	50611	129594	3.61%	0.444%
55	16.756	2490	2494	2503	rBV2	81165	151399	4.21%	0.519%
56	17.180	2562	2566	2573	rVB	58901	108785	3.03%	0.373%
57	17.327	2586	2591	2601	rVB9	48412	127031	3.54%	0.435%

Sum of corrected areas: 29190771

LSC Report - Integrated Chromatogram

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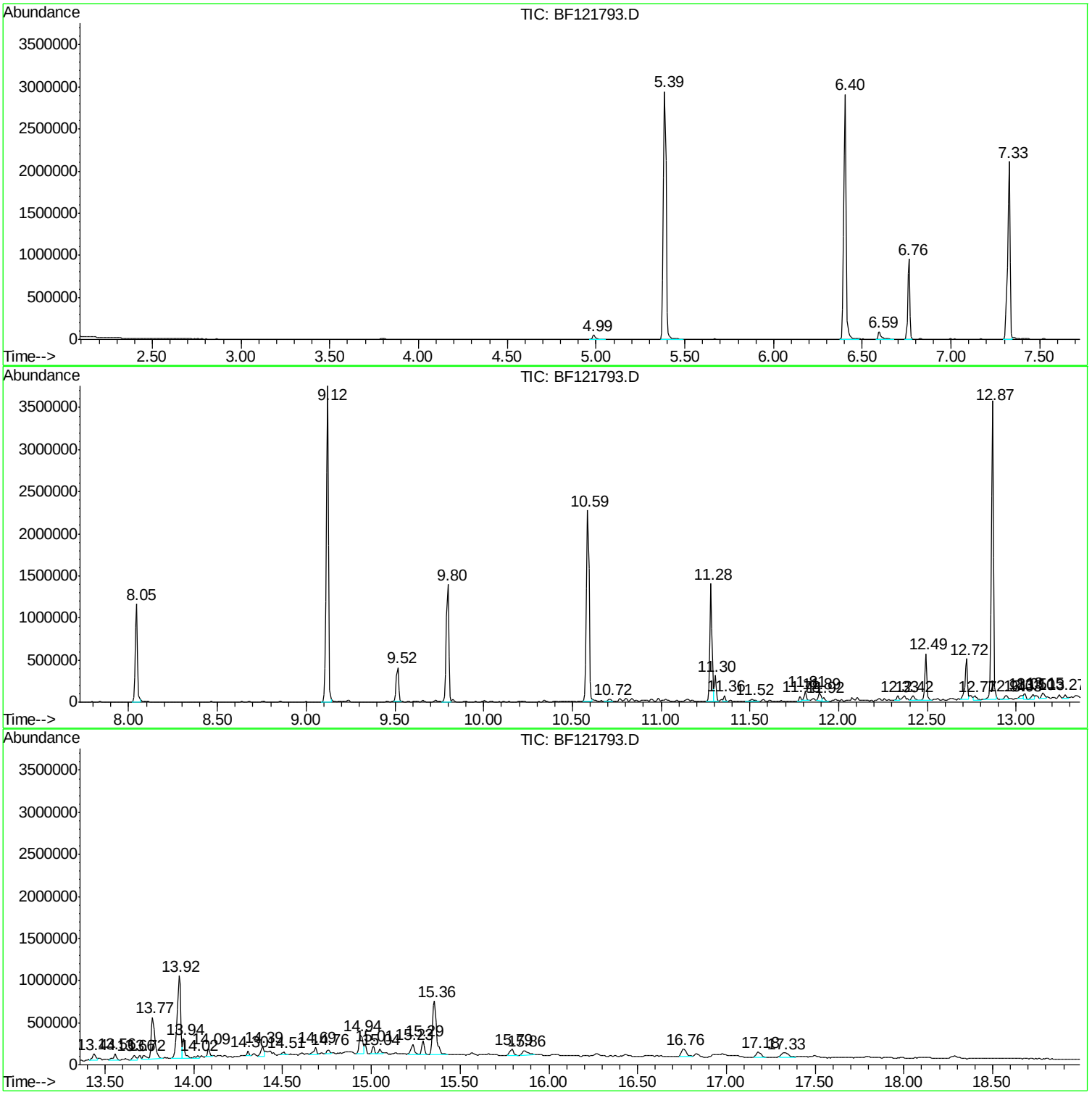
Data File : BF121793.D
Acq On : 2 Oct 2020 14:38
Operator : JU/CG
Sample : L4198-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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\BF100220\
Data File : BF121793.D
Acq On : 2 Oct 2020 14:38
Operator : JU/CG
Sample : L4198-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

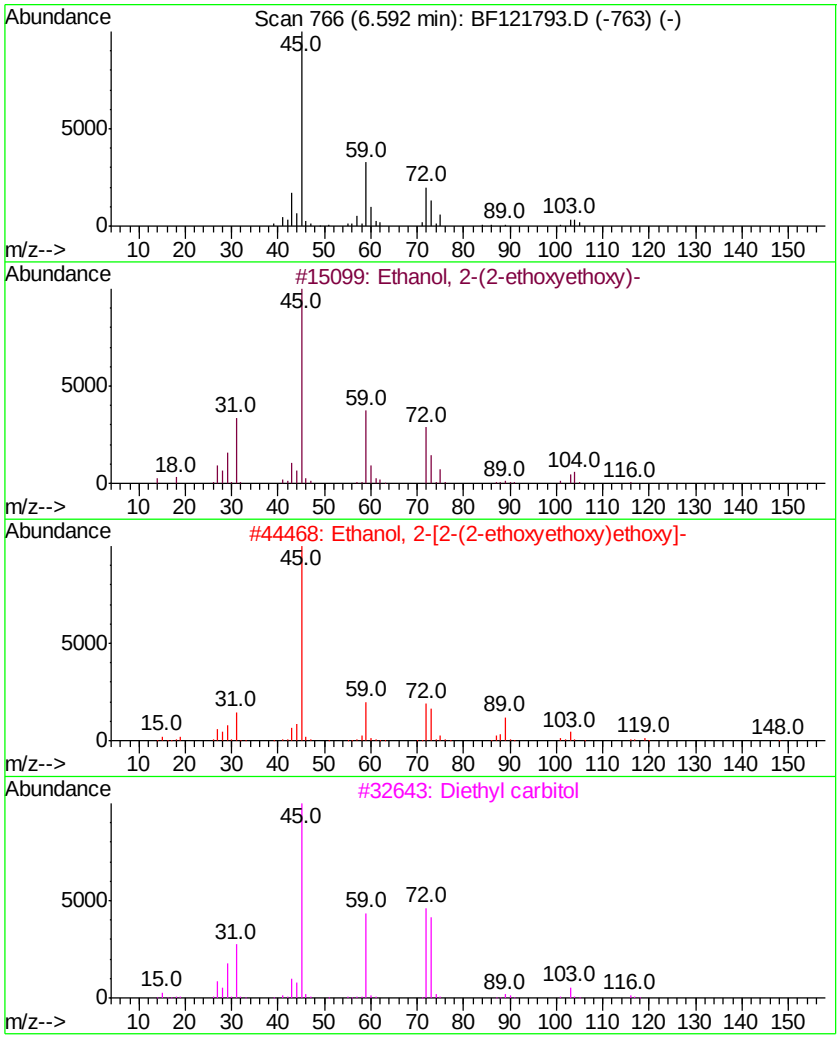
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

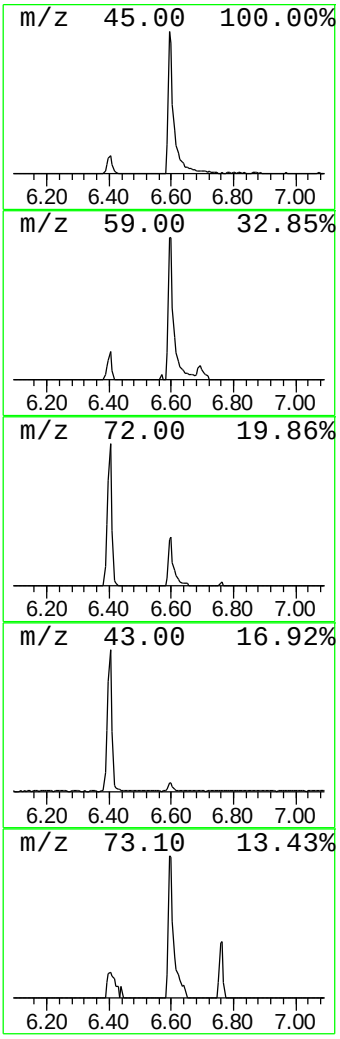
****

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	2.88 ng	114587	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	64
3	Diethyl carbitol	162	C8H18O3	000112-36-7	56
4	Methoxymethyl isothiocyanate	103	C3H5NOS	019900-84-6	53
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100220\
Data File : BF121793.D
Acq On : 2 Oct 2020 14:38
Operator : JU/CG
Sample : L4198-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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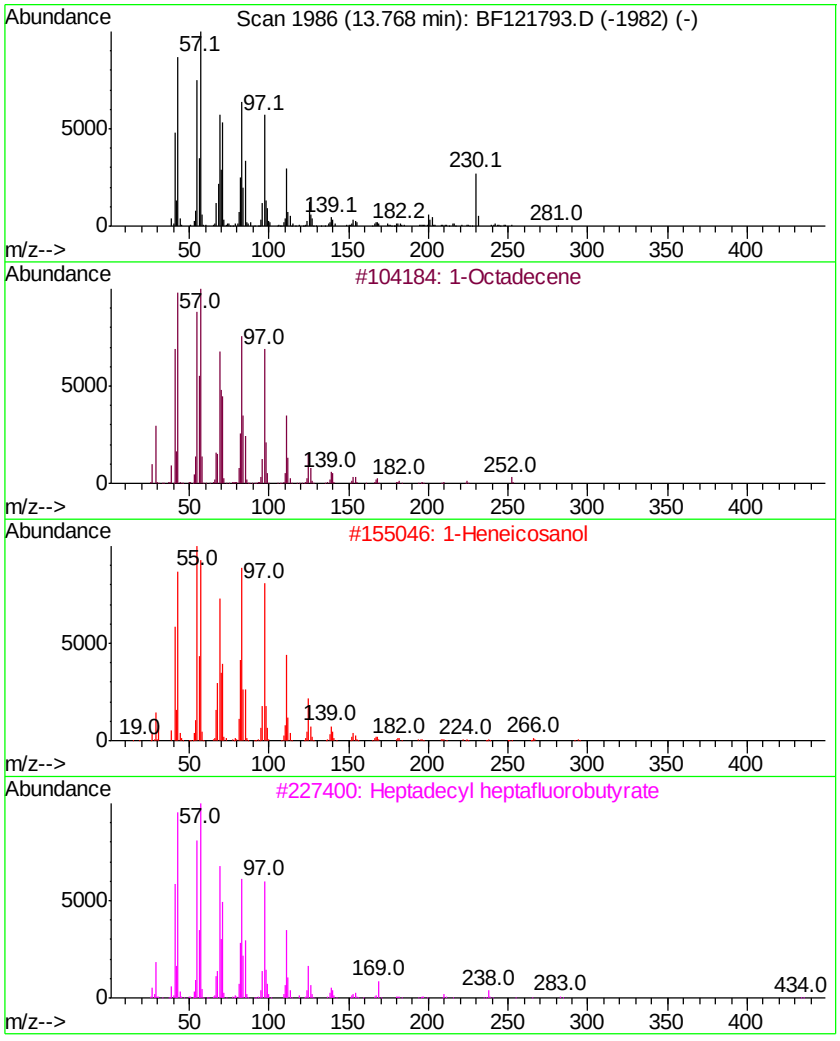
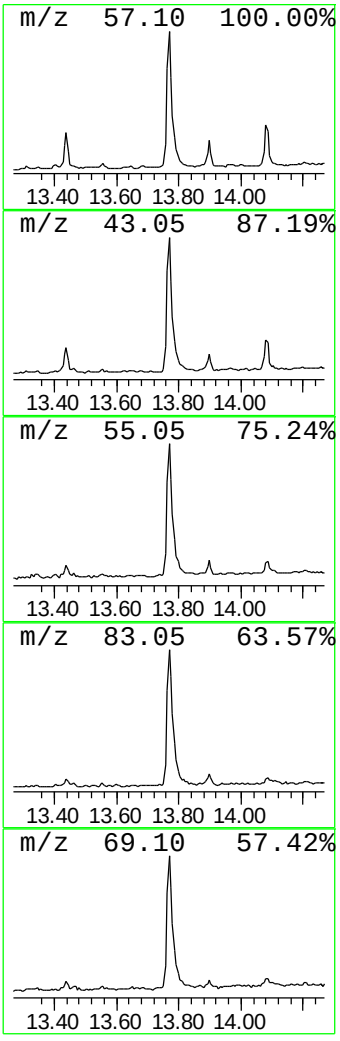
Peak Number 2 1-Octadecene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	10.06 ng	636938	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	97
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100220\
Data File : BF121793.D
Acq On : 2 Oct 2020 14:38
Operator : JU/CG
Sample : L4198-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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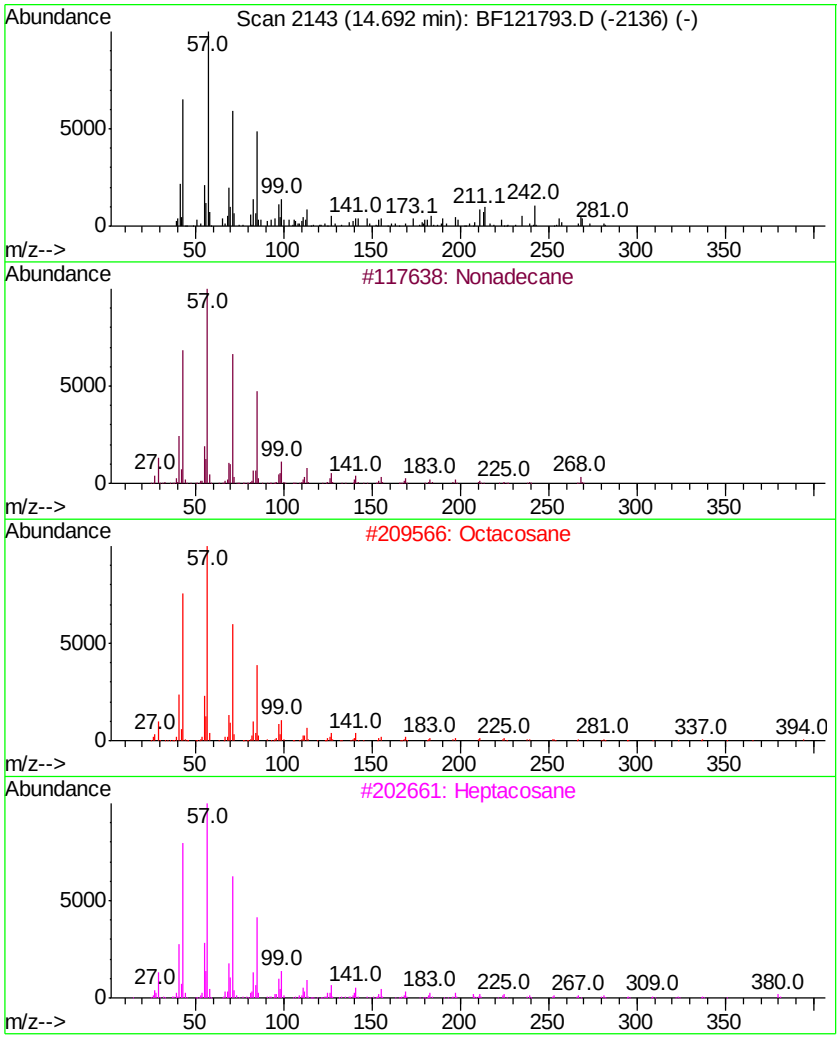
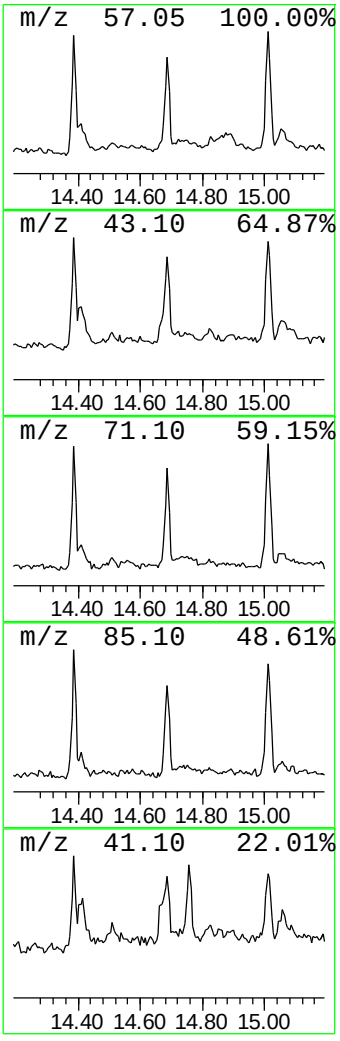
Peak Number 3 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.37 ng	109582	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Hexatriacontane	507	C36H74	000630-06-8	87





Library Search Compound Report

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Data File : BF121793.D
Acq On : 2 Oct 2020 14:38
Operator : JU/CG
Sample : L4198-13
Misc :
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Instrument : BNA_F
ClientSampleId : RO-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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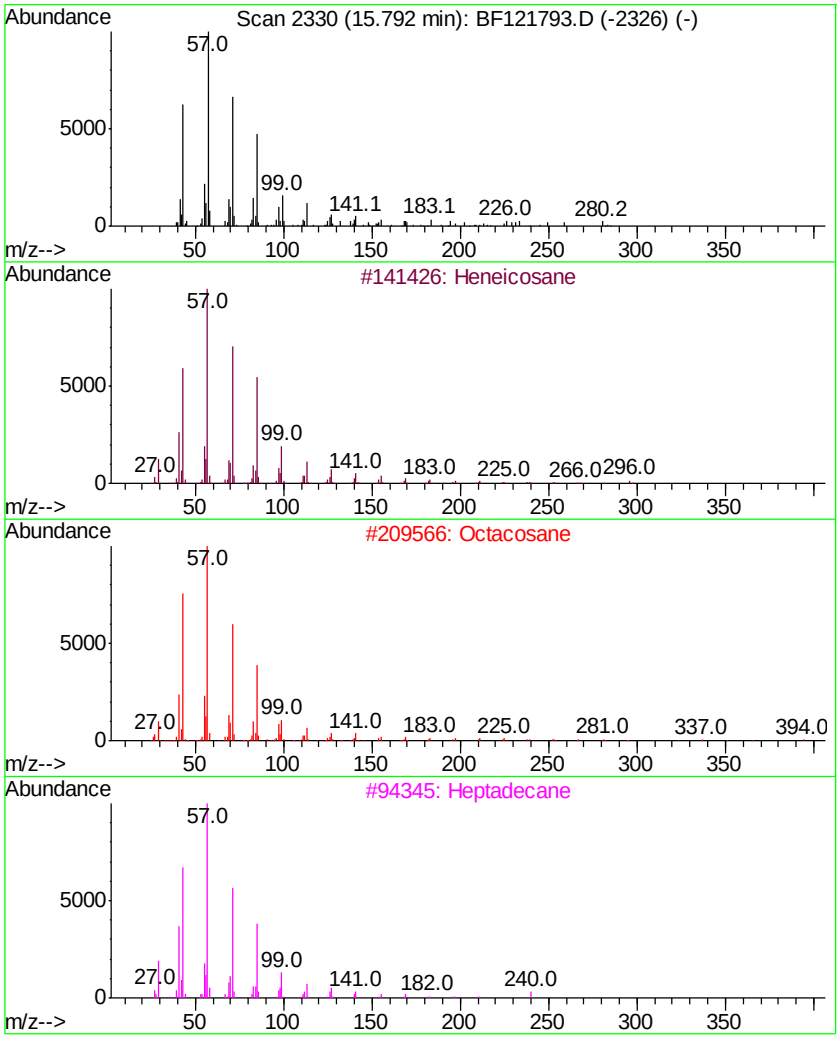
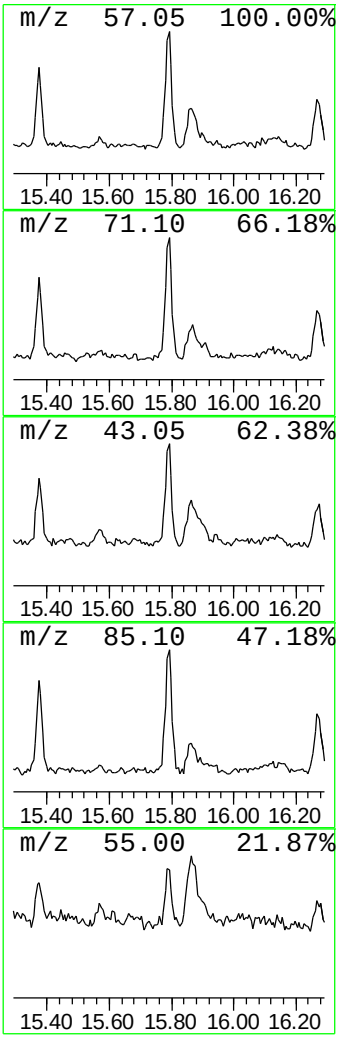
Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.25 ng	103879	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptadecane	240	C17H36	000629-78-7	87
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	87
5	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	87





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : RO-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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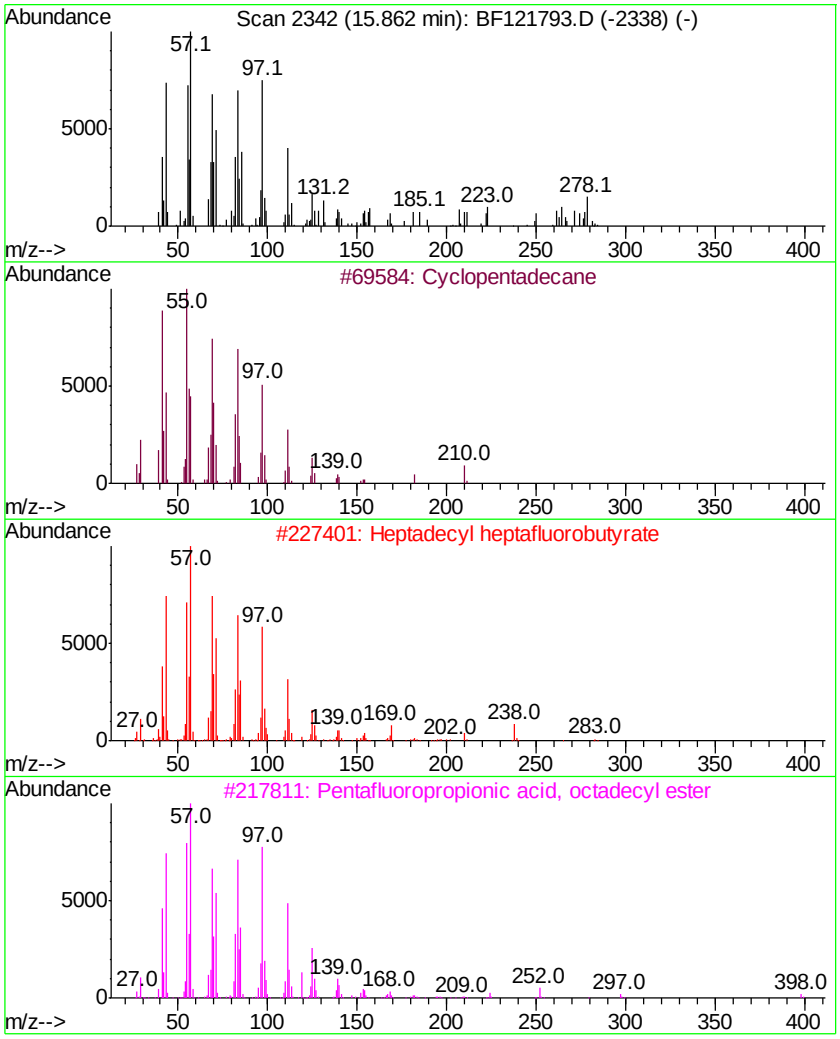
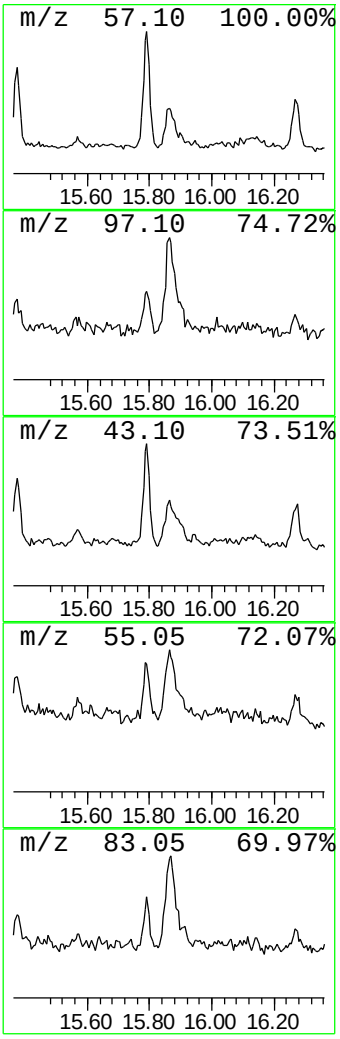
Peak Number 6 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	2.81 ng	129594	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90
4	Octacosanol	410	C28H58O	000557-61-9	90
5	Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	90





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Instrument : BNA_F
ClientSampleId : RO-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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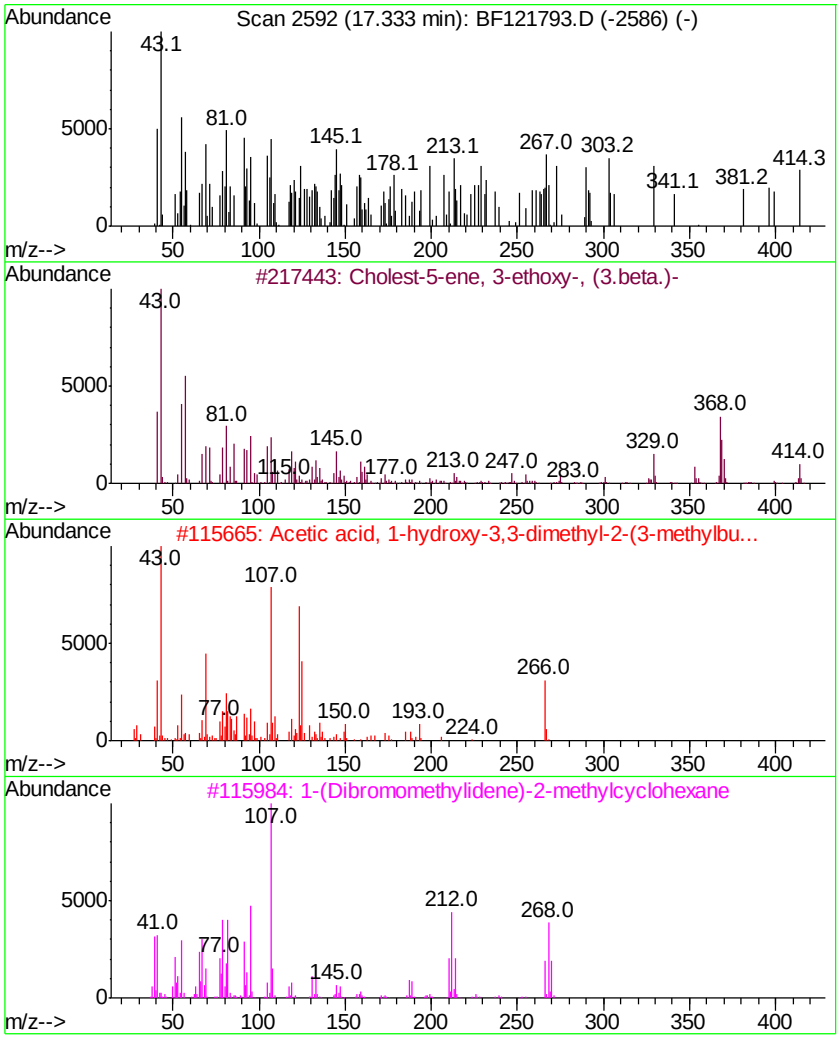
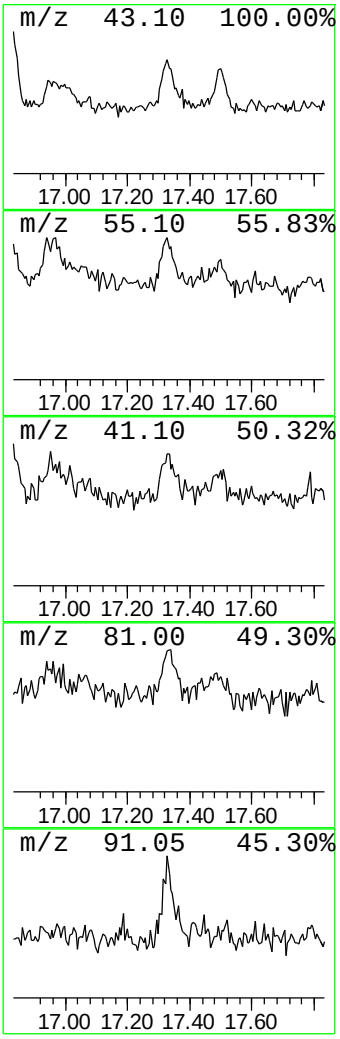
Peak Number 7 unknown17.33 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.33	2.75 ng	127031	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	27
2	Acetic acid, 1-hydroxy-3,3-dimet...	266	C16H26O3	1000188-31-1	14
3	1-(Dibromomethylidene)-2-methylc...	266	C8H12Br2	1000305-56-5	14
4	5-Benzylcarbamoyl-1H-imidazole-4...	273	C14H15N3O3	312758-83-1	11
5	Quinoline-2-carboxylic acid (pyr...	263	C16H13N3O	1000302-58-7	10





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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
Ethanol, 2-(2-eth...	6.59	2.9	ng	114587	1	6.76	796757	20.0
1-Octadecene	13.77	10.1	ng	636938	5	13.92	1266770	20.0
Nonadecane	14.69	2.4	ng	109582	6	15.36	922808	20.0
Heneicosane	15.79	2.3	ng	103879	6	15.36	922808	20.0
Cyclopentadecane	15.86	2.8	ng	129594	6	15.36	922808	20.0
unknown17.33	17.33	2.8	ng	127031	6	15.36	922808	20.0