LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102821\
Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-GS

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-BF102521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125984.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	15	rVB	2964644	3731991	89.82%	9.855%
2	5.469	570	575	578	rBV	4126017	4155154	100.00%	10.972%
3	6.481	741	747	750	rBV	4128204	4073044	98.02%	10.755%
4	6.857	807	811	814	rBV	1367257	1065107	25.63%	2.812%
5	7.416	901	906	909	rBV	3015439	2668474	64.22%	7.046%
6	8.040	1009	1012	1025	rBV	761498	846498	20.37%	2.235%
7	8.140	1025	1029	1032	rBV	1667604	1356510	32.65%	3.582%
8	9.216	1207	1212	1215	rBV	4484540	3888914	93.59%	10.269%
9	9.751	1300	1303	1307	rVB	63774	51856	1.25%	0.137%
10	9.892	1323	1327	1330	rBV	1725786	1378725	33.18%	3.641%
11	10.675	1456	1460	1466	rBV	2616772	2352431	56.61%	6.212%
12	11.375	1575	1579	1581	rBV	1610289	1272298	30.62%	3.360%
13	11.398	1581	1583	1586	rVV	220177	167275	4.03%	0.442%
14	11.445	1586	1591	1595	rVB2	65406	69983	1.68%	0.185%
15	11.775	1643	1647	1654	rBV3	54310	72871	1.75%	0.192%
16	11.875	1661	1664	1666	rBV	120476	108070	2.60%	0.285%
17	11.904	1666	1669	1673	rVB	362535	299639	7.21%	0.791%
18	11.986	1679	1683	1685	rBV	155933	150428	3.62%	0.397%
19	12.010	1685	1687	1691	rVB	111381	93325	2.25%	0.246%
20	12.169	1712	1714	1716	rBV	50817	47440	1.14%	0.125%
21	12.192	1716	1718	1722	rVB4	51183	50887	1.22%	0.134%
22	12.351	1743	1745	1747	rBV	56662	42837	1.03%	0.113%
23	12.427	1752	1758	1761	rBV	169109	187629	4.52%	0.495%
24	12.463	1761	1764	1766	rVV3	74169	101322	2.44%	0.268%
25	12.510	1769	1772	1777	rBV4	61624	82652	1.99%	0.218%
26	12.586	1781	1785	1789	rVB	400755	332645	8.01%	0.878%
27	12.686	1799	1802	1804	rBV2	55794	59050	1.42%	0.156%
28	12.816	1818	1824	1826	rBV	437101	449369	10.81%	1.187%
29	12.869	1830	1833	1837	rVB2	71278	95093	2.29%	0.251%
30	12.963	1845	1849	1852	rBV	3654679	3085543	74.26%	8.148%
31	13.033	1857	1861	1864	rBV4	83276	108372	2.61%	0.286%
32	13.122	1873	1876	1877	rBV2	58011	55214	1.33%	0.146%
33	13.139	1877	1879	1882	rVB2	120309	120337	2.90%	0.318%
34	13.204	1885	1890	1894	rBV2	93830	132333	3.18%	0.349%
35	13.245	1894	1897	1900	rBV2	111468	101085	2.43%	0.267%
36	13.339	1910	1913	1915	rVB	109284	80413	1.94%	0.212%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102821\
Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-GS

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-BF102521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.369	1915	1918	1922	rVB	107461	87576	2.11%	0.231%
38	13.445	1929	1931	1936	rVB6	35135	50622	1.22%	0.134%
39	13.545	1945	1948	1950	rBV2	86060	85096	2.05%	0.225%
40	13.645	1963	1965	1970	rVB3	58525	83436	2.01%	0.220%
41	13.751	1980	1983	1985	rBV3	59215	77321	1.86%	0.204%
42	13.874	2001	2004	2013	rVB2	335416	495428	11.92%	1.308%
43	14.010	2022	2027	2030	rBV2	1326158	1413507	34.02%	3.732%
44	14.033	2030	2031	2039	rVB	241138	212212	5.11%	0.560%
45	14.186	2055	2057	2062	rVB2	86704	77010	1.85%	0.203%
46	14.398	2089	2093	2096	rBV2	110398	132944	3.20%	0.351%
47	14.433	2096	2099	2102	rVB	68478	59007	1.42%	0.156%
48	14.492	2106	2109	2111	rBV2	133954	108695	2.62%	0.287%
49	14.521	2111	2114	2116	rBV	104489	110532	2.66%	0.292%
50	14.804	2160	2162	2169	rVB2	80251	118946	2.86%	0.314%
51	15.051	2200	2204	2207	rBV	155959	252287	6.07%	0.666%
52	15.145	2217	2220	2226	rVB2	83319	124676	3.00%	0.329%
53	15.351	2251	2255	2258	rVB	114444	134038	3.23%	0.354%
54	15.410	2262	2265	2271	rBV	157963	188348	4.53%	0.497%
55	15.474	2272	2276	2280	rBV2	879675	1071384	25.78%	2.829%
56	15.963	2357	2359	2364	rVB3	47446	52785	1.27%	0.139%

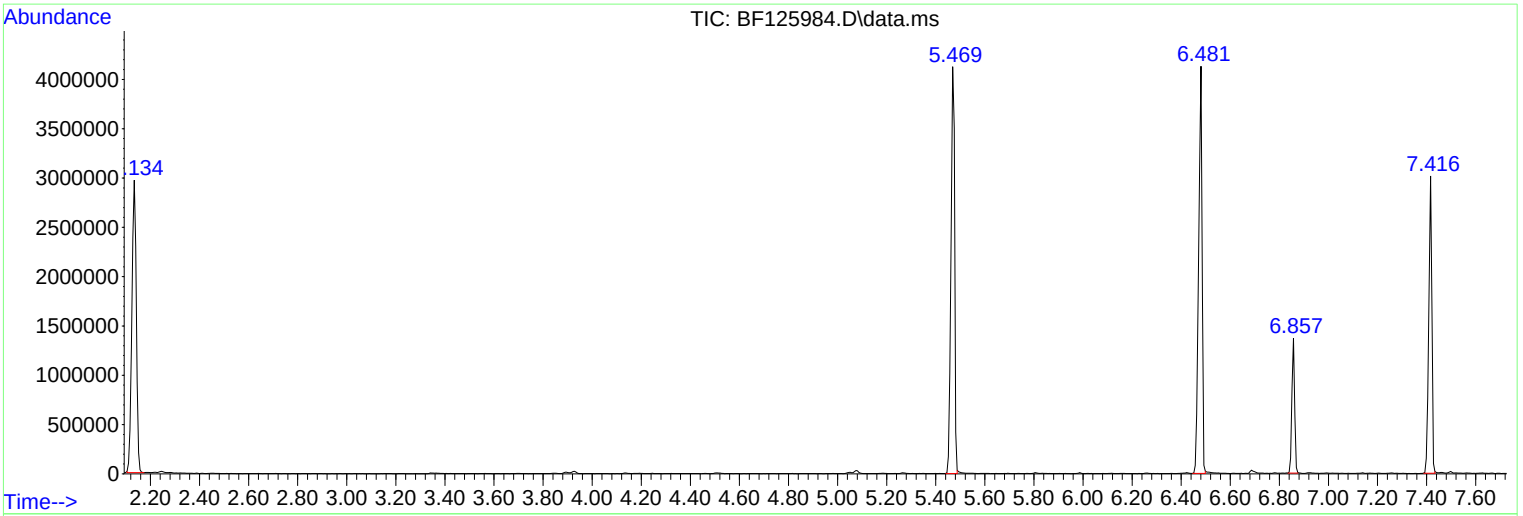
Sum of corrected areas: 37870664

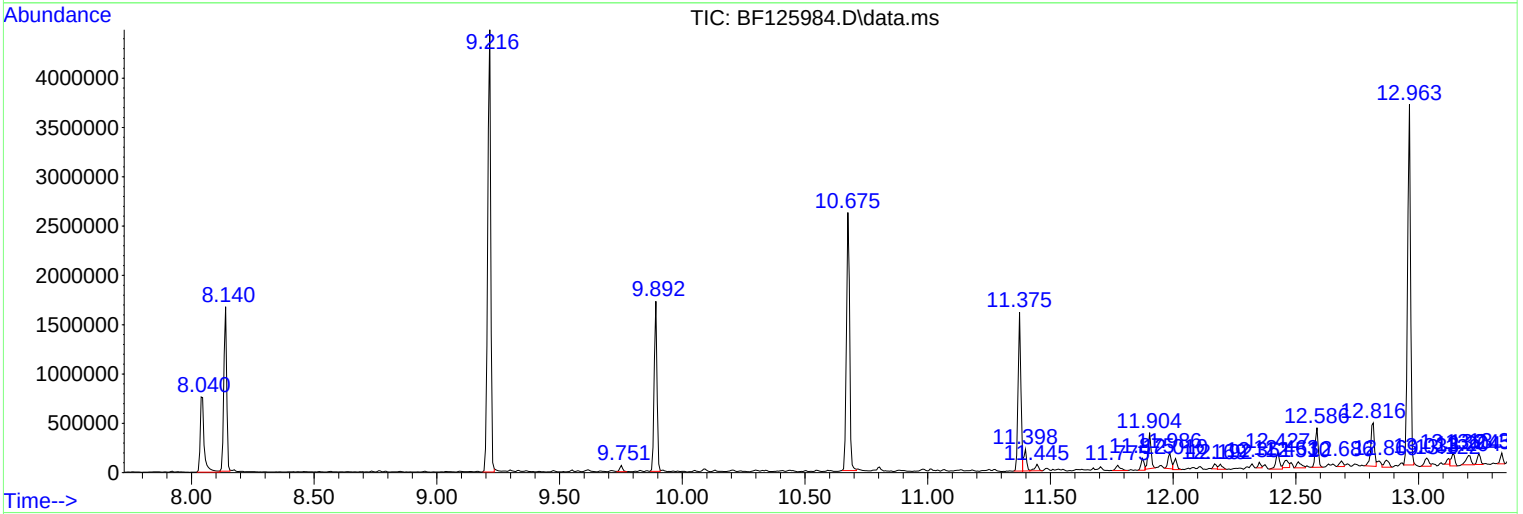
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102821\
Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

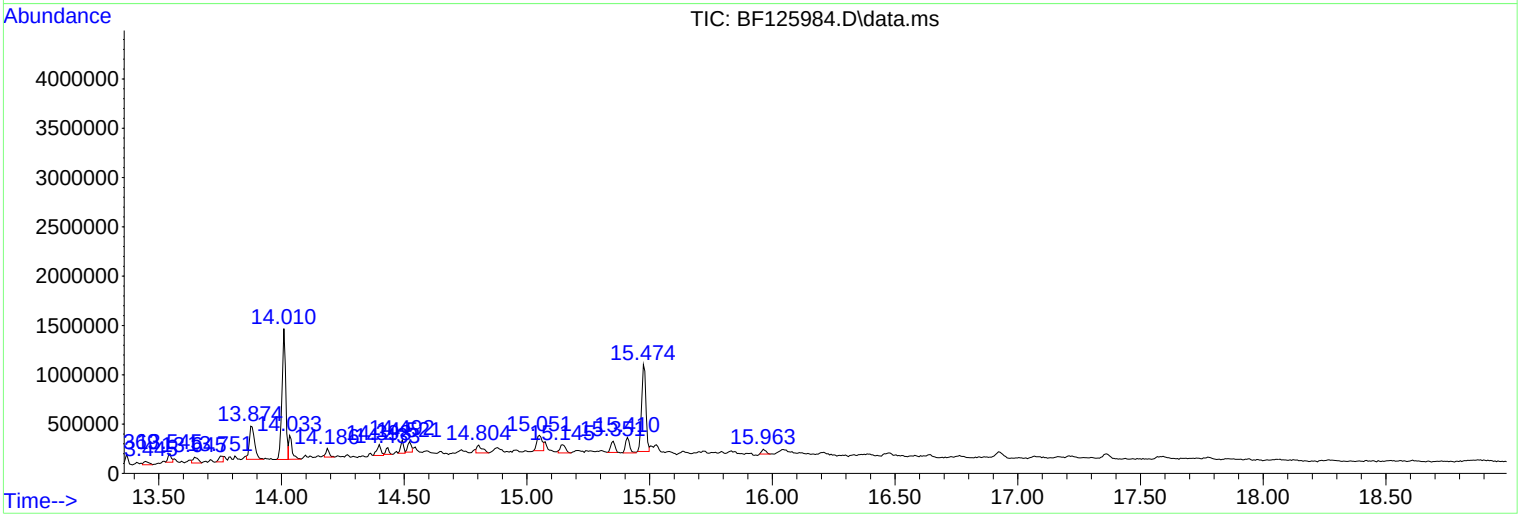
Instrument :
BNA_F
ClientSampleId :
TH-GS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.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\BF102821\
Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

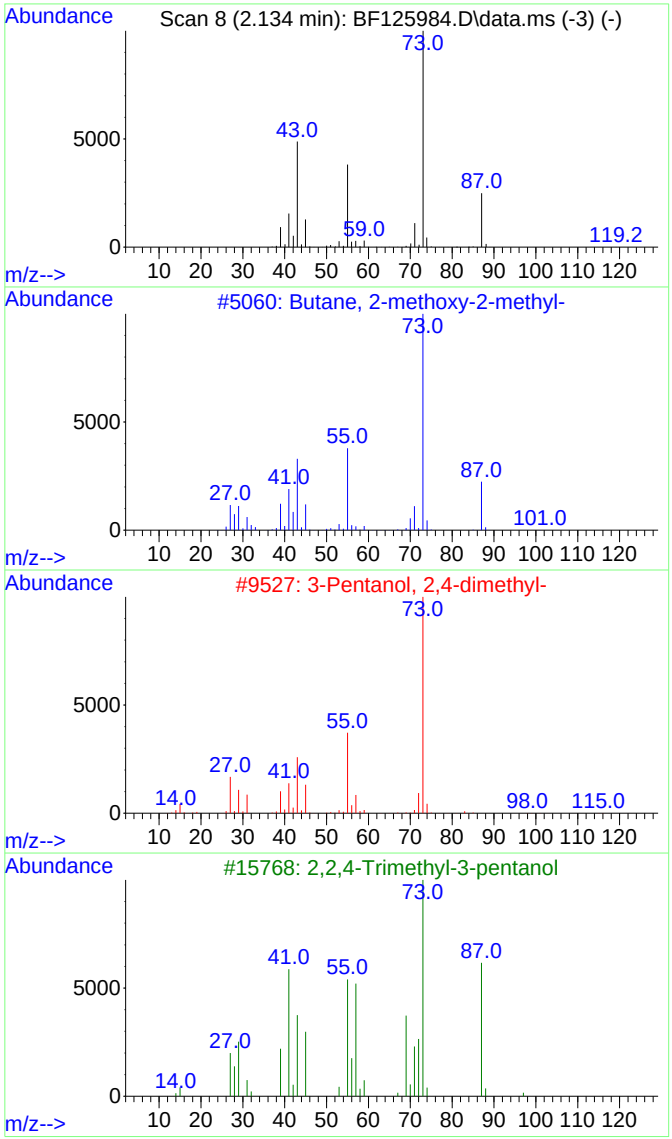
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

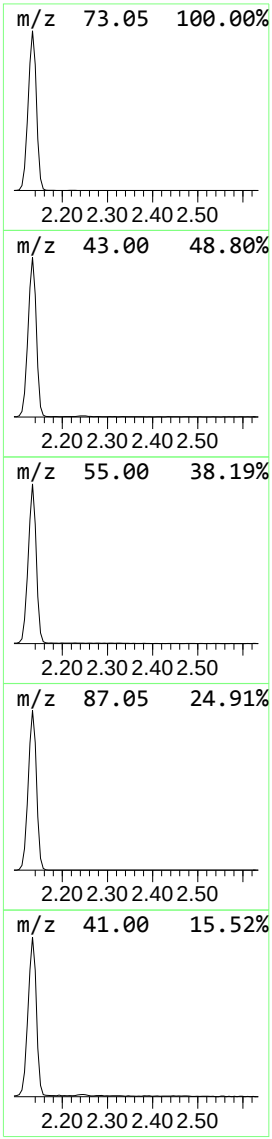
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	70.08 ng	3731990	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102821\
Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-GS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

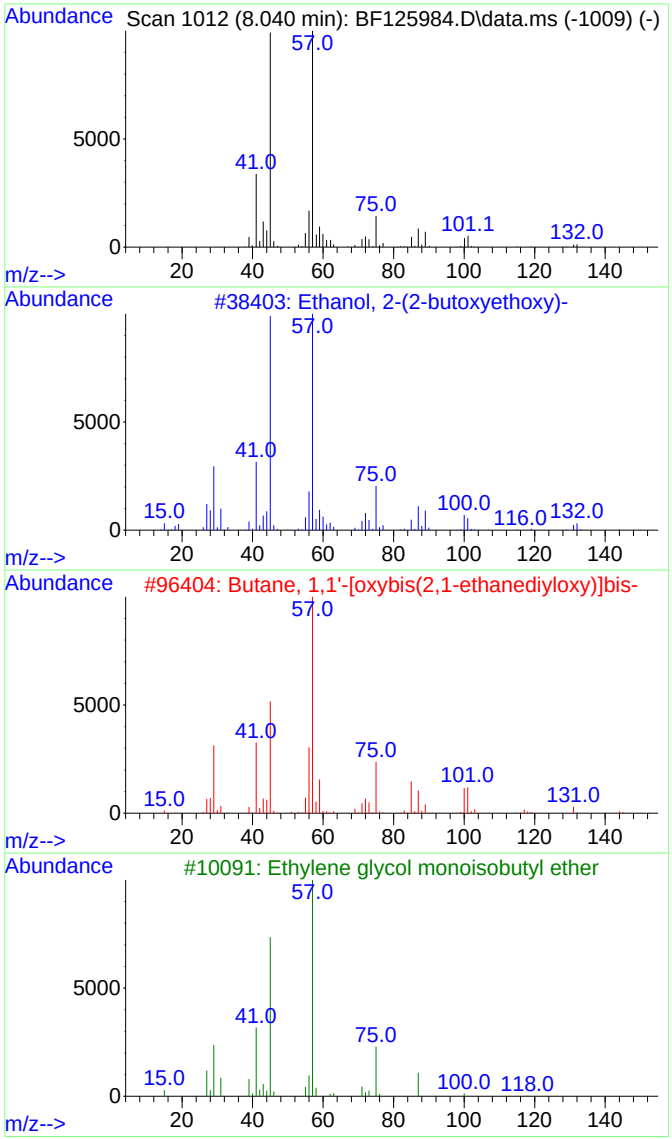
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

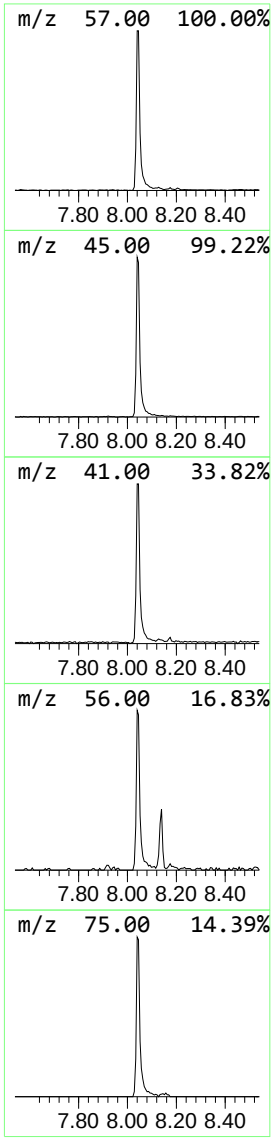
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.040	12.48 ng	846498	Naphthalene-d8	8.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	64
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





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Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-GS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

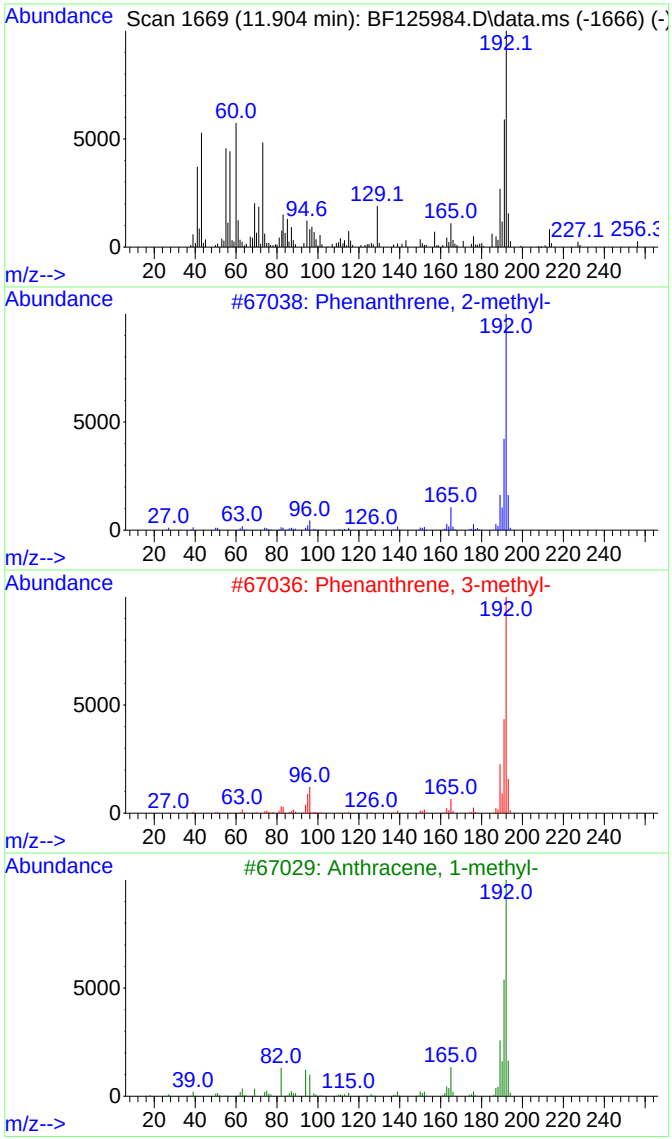
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

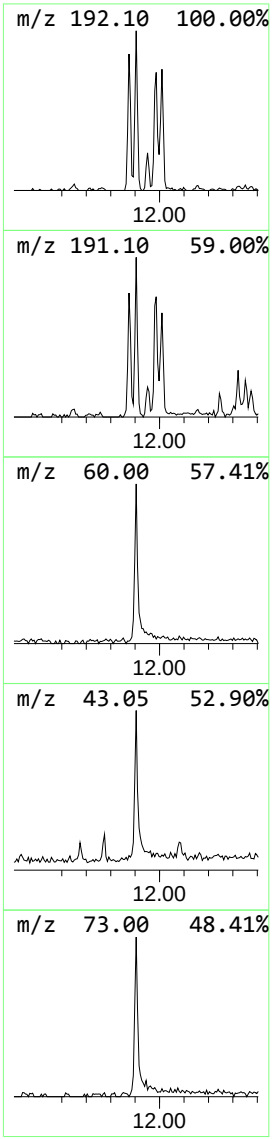
****

Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	4.71 ng	299639	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
2	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	83
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	78
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	70
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102821\
Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-GS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

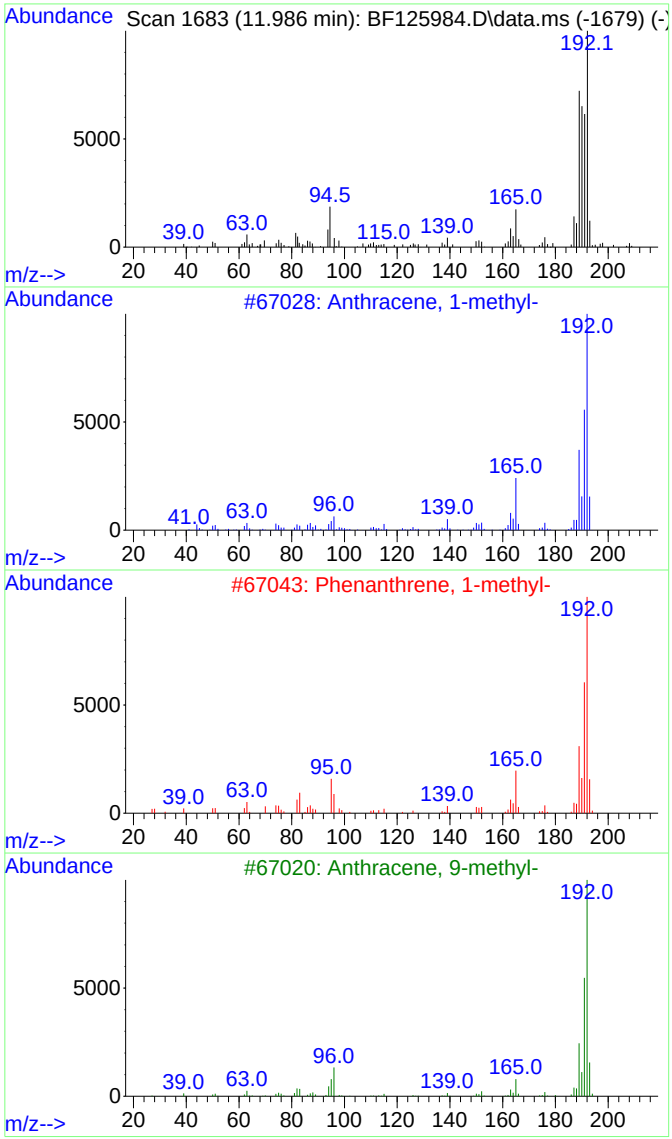
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

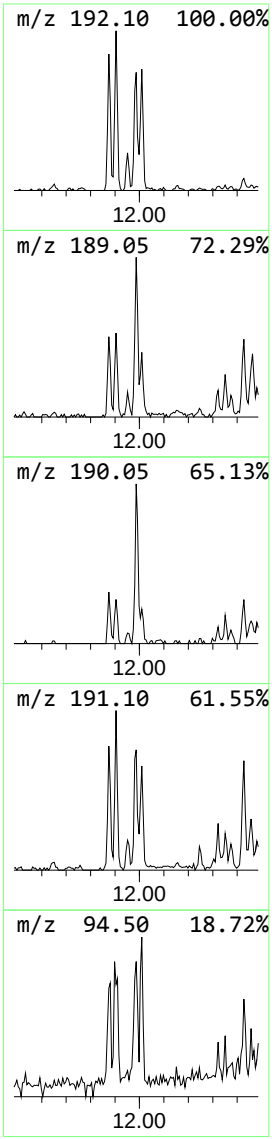
****

Peak Number 4 Anthracene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.986	2.36 ng	150428	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	89
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	70
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	60
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	50
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102821\
Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-GS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

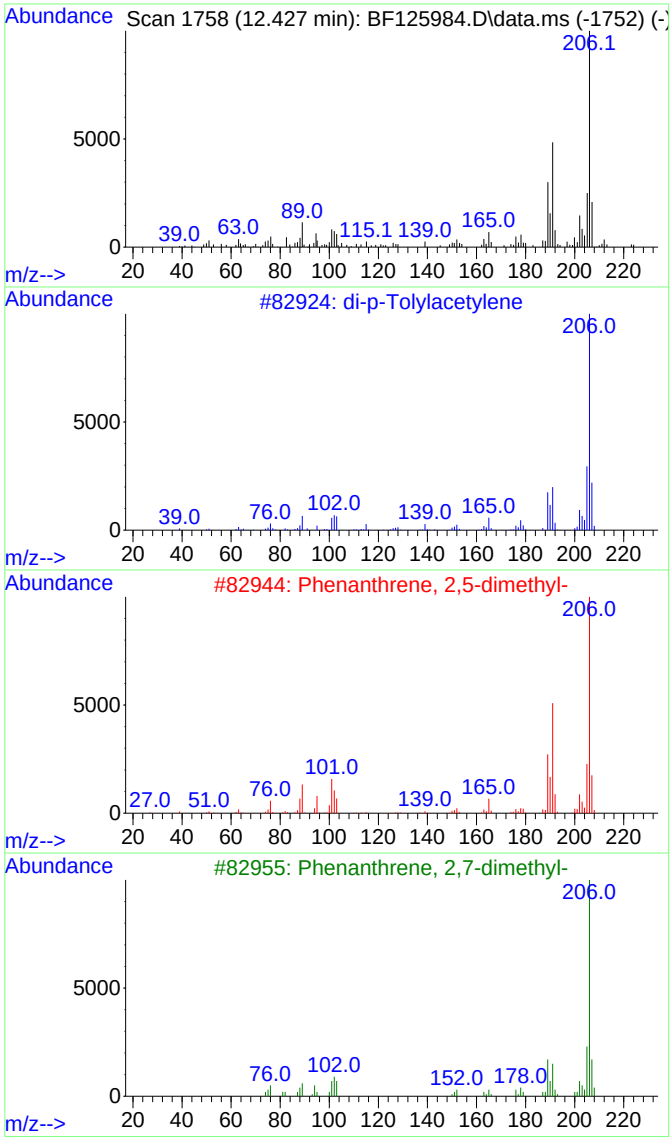
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

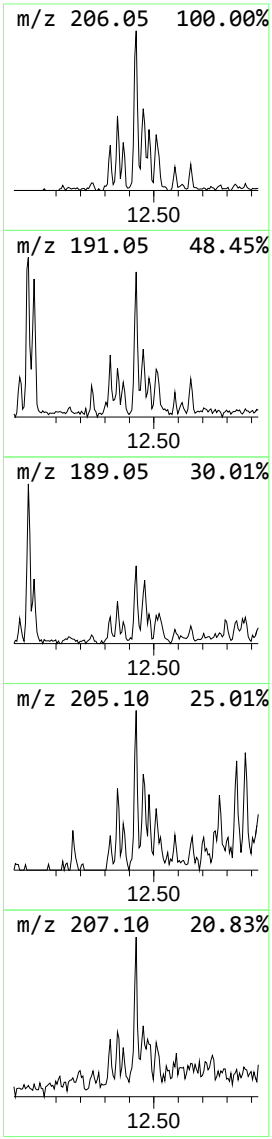
****

Peak Number 5 di-p-Tolylacetylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.428	2.95 ng	187629	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	di-p-Tolylacetylene	206	C16H14	002789-88-0	93
2	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
3	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	92
4	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91
5	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	89





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Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-GS

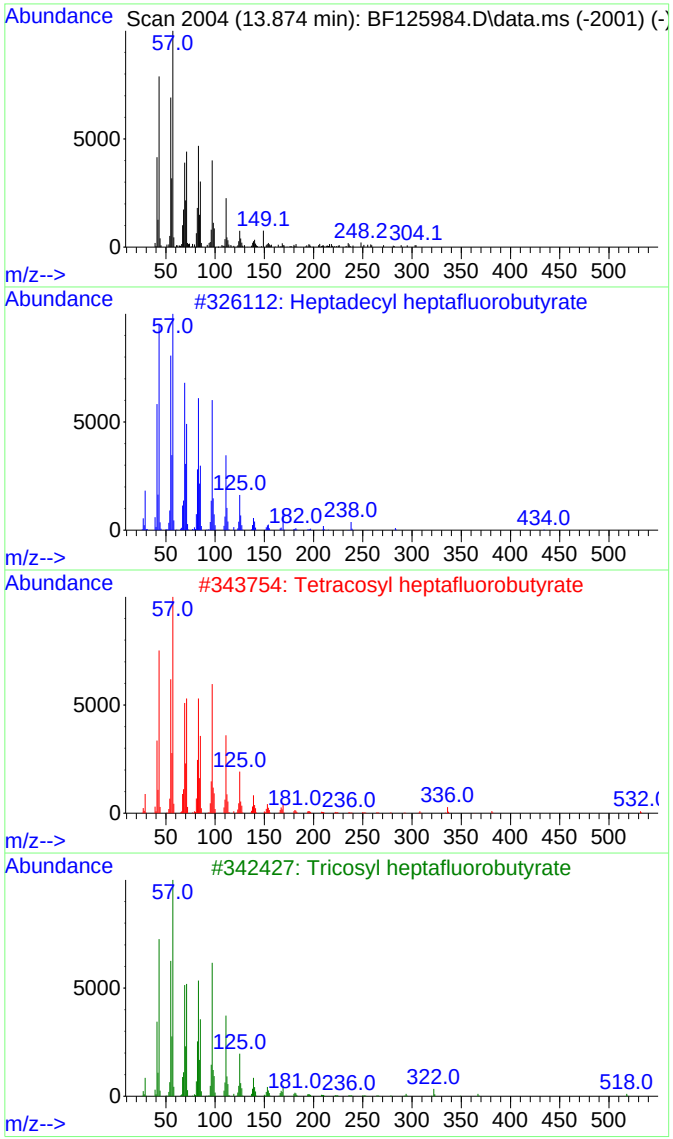
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

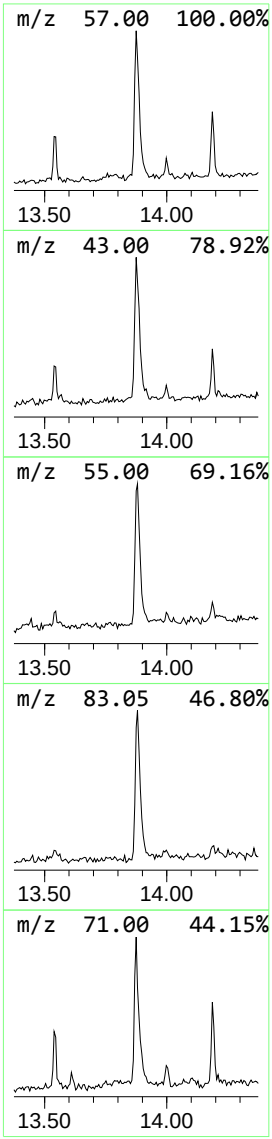
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	7.01 ng	495428	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102821\
Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-GS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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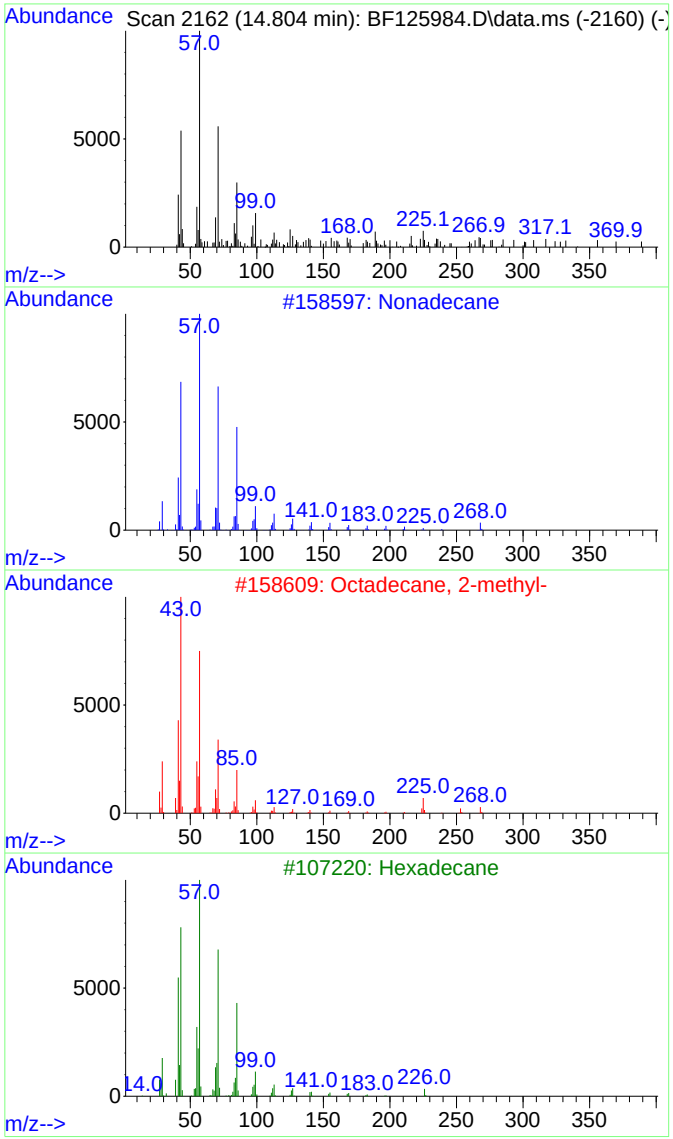
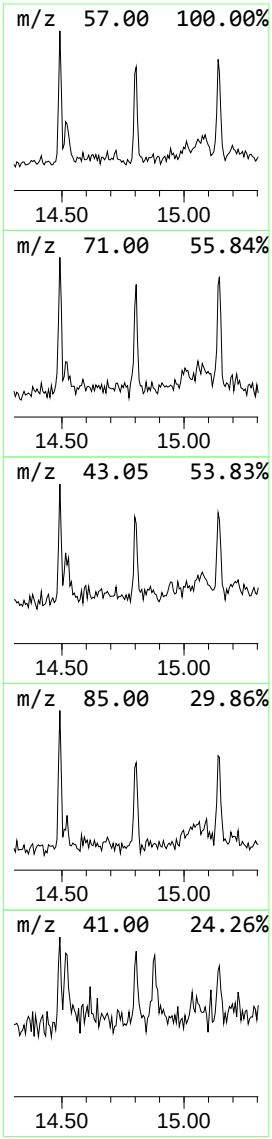
Peak Number 7 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	2.22 ng	118946	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	64
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	64
3	Hexadecane	226	C16H34	000544-76-3	53
4	Tricosane	324	C23H48	000638-67-5	53
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	49





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Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TH-GS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

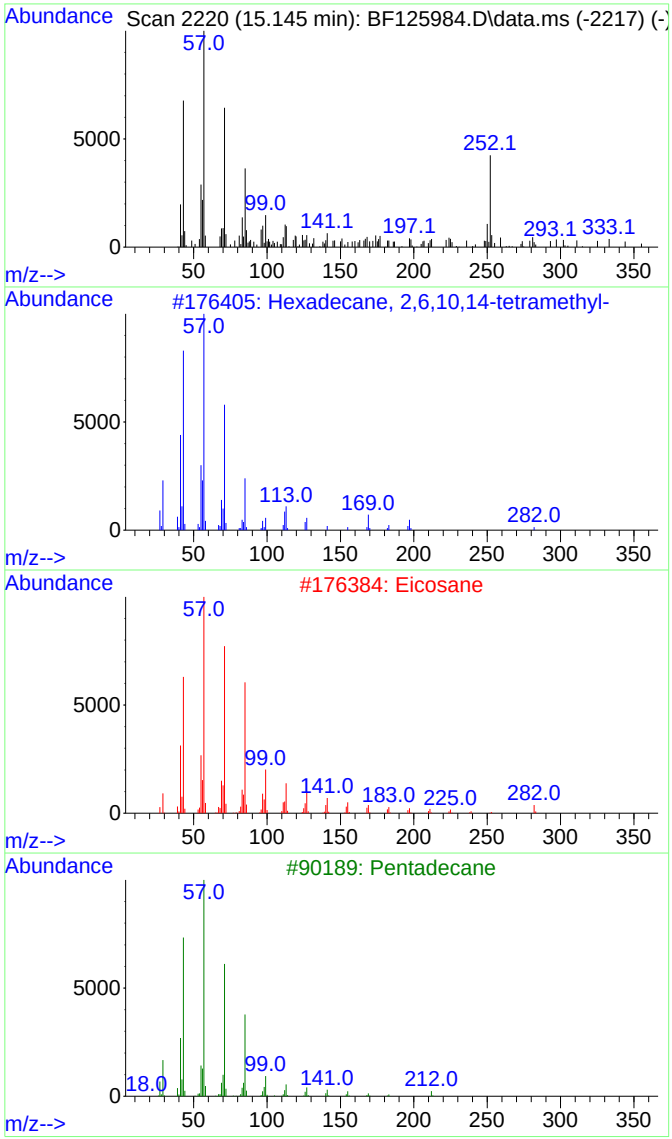
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

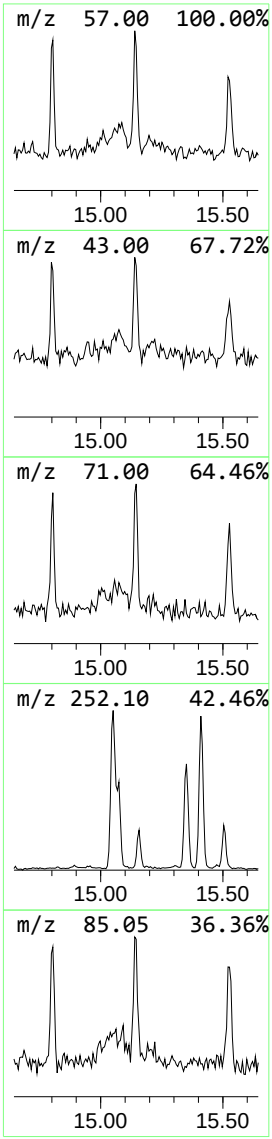
****

Peak Number 8 Hexadecane, 2,6,10,14-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	2.33 ng	124676	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	56
2	Eicosane	282	C20H42	000112-95-8	56
3	Pentadecane	212	C15H32	000629-62-9	46
4	Hexadecane	226	C16H34	000544-76-3	42
5	2,6-Dimethyldecane	170	C12H26	013150-81-7	42





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102821\
Data File : BF125984.D
Acq On : 28 Oct 2021 12:36
Operator : JU/CG
Sample : M4358-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TH-GS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.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...	2.134	70.1	ng	3731990	1	6.857	1065110	20.0
Ethanol, 2-(2-b...	8.040	12.5	ng	846498	2	8.140	1356510	20.0
Phenanthrene, 2...	11.904	4.7	ng	299639	4	11.375	1272300	20.0
Anthracene, 1-m...	11.986	2.4	ng	150428	4	11.375	1272300	20.0
di-p-Tolylacety...	12.428	3.0	ng	187629	4	11.375	1272300	20.0
Heptadecyl hept...	13.874	7.0	ng	495428	5	14.010	1413510	20.0
Nonadecane	14.804	2.2	ng	118946	6	15.474	1071380	20.0
Hexadecane, 2,6...	15.145	2.3	ng	124676	6	15.474	1071380	20.0