LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125186.D
Acq On : 24 Aug 2021 15:38
Operator : JU/CG
Sample : M3467-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-4-(177.00)

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125186.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	14	20	28	rVB	692746	862820	29.67%	3.009%
2	5.134	511	518	525	rVB	120284	155630	5.35%	0.543%
3	5.528	580	585	588	rBV	2989350	2780722	95.63%	9.698%
4	6.534	751	756	759	rBV	3086232	2907756	100.00%	10.141%
5	6.916	817	821	824	rVB	1043372	884241	30.41%	3.084%
6	7.475	911	916	919	rBV	2299325	1984102	68.23%	6.920%
7	8.092	1018	1021	1035	rBV	432431	527425	18.14%	1.839%
8	8.198	1035	1039	1041	rVV	1316129	1184762	40.74%	4.132%
9	8.216	1041	1042	1045	rVB	52878	33620	1.16%	0.117%
10	9.269	1217	1221	1224	rBV	3337768	2713658	93.32%	9.464%
11	9.663	1285	1288	1295	rVB	104465	105457	3.63%	0.368%
12	9.810	1310	1313	1317	rVB	41180	34536	1.19%	0.120%
13	9.951	1333	1337	1340	rVB	1656453	1331130	45.78%	4.642%
14	10.151	1366	1371	1375	rBV2	34521	37969	1.31%	0.132%
15	10.739	1467	1471	1474	rBV	2320327	2152761	74.04%	7.508%
16	10.863	1487	1492	1496	rVB3	38450	55652	1.91%	0.194%
17	11.239	1553	1556	1560	rVB2	47870	38547	1.33%	0.134%
18	11.439	1586	1590	1592	rBV	1575029	1406175	48.36%	4.904%
19	11.457	1592	1593	1597	rVB	112440	87486	3.01%	0.305%
20	11.663	1623	1628	1630	rBV2	41097	44633	1.53%	0.156%
21	11.822	1652	1655	1658	rBV3	48616	39083	1.34%	0.136%
22	11.957	1671	1678	1683	rBV2	336794	406544	13.98%	1.418%
23	12.045	1690	1693	1696	rBV2	58087	60327	2.07%	0.210%
24	12.133	1701	1708	1712	rBV7	20047	48683	1.67%	0.170%
25	12.257	1726	1729	1733	rVB2	72341	67661	2.33%	0.236%
26	12.380	1744	1750	1752	rBV5	43574	45014	1.55%	0.157%
27	12.410	1752	1755	1758	rVV	62546	51090	1.76%	0.178%
28	12.486	1765	1768	1771	rBV	92863	84486	2.91%	0.295%
29	12.569	1780	1782	1788	rBV3	58155	63808	2.19%	0.223%
30	12.651	1792	1796	1799	rBV	560191	459949	15.82%	1.604%
31	12.739	1808	1811	1814	rBV2	92906	81924	2.82%	0.286%
32	12.880	1832	1835	1840	rVB	527582	453289	15.59%	1.581%
33	12.933	1840	1844	1848	rVB2	36430	52532	1.81%	0.183%
34	13.021	1855	1859	1866	rVB	2617944	2240035	77.04%	7.812%
35	13.092	1868	1871	1875	rBV3	65619	96259	3.31%	0.336%
36	13.180	1883	1886	1889	rBV4	48984	68309	2.35%	0.238%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125186.D
Acq On : 24 Aug 2021 15:38
Operator : JU/CG
Sample : M3467-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-4-(177.00)

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.310	1904	1908	1911	rVB2	83809	84125	2.89%	0.293%
38	13.404	1921	1924	1926	rBV	61016	51835	1.78%	0.181%
39	13.433	1926	1929	1933	rVV2	44446	50100	1.72%	0.175%
40	13.710	1970	1976	1982	rBV	100285	115581	3.97%	0.403%
41	13.827	1991	1996	1999	rBV2	54834	85314	2.93%	0.298%
42	13.857	1999	2001	2003	rBV	56432	58481	2.01%	0.204%
43	13.874	2003	2004	2008	rVB2	56327	46830	1.61%	0.163%
44	13.916	2008	2011	2014	rBV2	72050	75690	2.60%	0.264%
45	13.945	2014	2016	2017	rBV	57539	47367	1.63%	0.165%
46	13.968	2017	2020	2023	rVV3	30112	42621	1.47%	0.149%
47	14.080	2034	2039	2041	rBV2	1126244	1233795	42.43%	4.303%
48	14.104	2041	2043	2050	rVB	299996	279252	9.60%	0.974%
49	14.204	2058	2060	2062	rBV2	34778	35474	1.22%	0.124%
50	14.292	2072	2075	2079	rBV3	24227	40402	1.39%	0.141%
51	14.463	2100	2104	2107	rVB	75870	76845	2.64%	0.268%
52	14.498	2107	2110	2114	rVB2	73901	65841	2.26%	0.230%
53	14.545	2115	2118	2122	rVB4	38678	58816	2.02%	0.205%
54	14.592	2123	2126	2128	rBV	44374	42065	1.45%	0.147%
55	14.663	2136	2138	2144	rVB	36348	40939	1.41%	0.143%
56	14.857	2169	2171	2176	rVB3	28717	37015	1.27%	0.129%
57	14.939	2181	2185	2189	rBV2	59516	86435	2.97%	0.301%
58	15.033	2198	2201	2205	rBV3	39363	39477	1.36%	0.138%
59	15.127	2213	2217	2221	rBV2	279400	453343	15.59%	1.581%
60	15.210	2227	2231	2234	rBV2	44695	50030	1.72%	0.174%
61	15.245	2234	2237	2240	rVB	43776	48403	1.66%	0.169%
62	15.445	2267	2271	2277	rVB	164059	209806	7.22%	0.732%
63	15.504	2277	2281	2287	rVB	133324	175411	6.03%	0.612%
64	15.574	2288	2293	2297	rBV	806572	1014249	34.88%	3.537%
65	16.580	2459	2464	2467	rBV3	27232	45349	1.56%	0.158%
66	17.074	2543	2548	2556	rBV2	76182	145298	5.00%	0.507%
67	17.139	2556	2559	2564	rBV4	31785	52920	1.82%	0.185%
68	17.527	2620	2625	2634	rVB	67092	136440	4.69%	0.476%

Sum of corrected areas: 28673624

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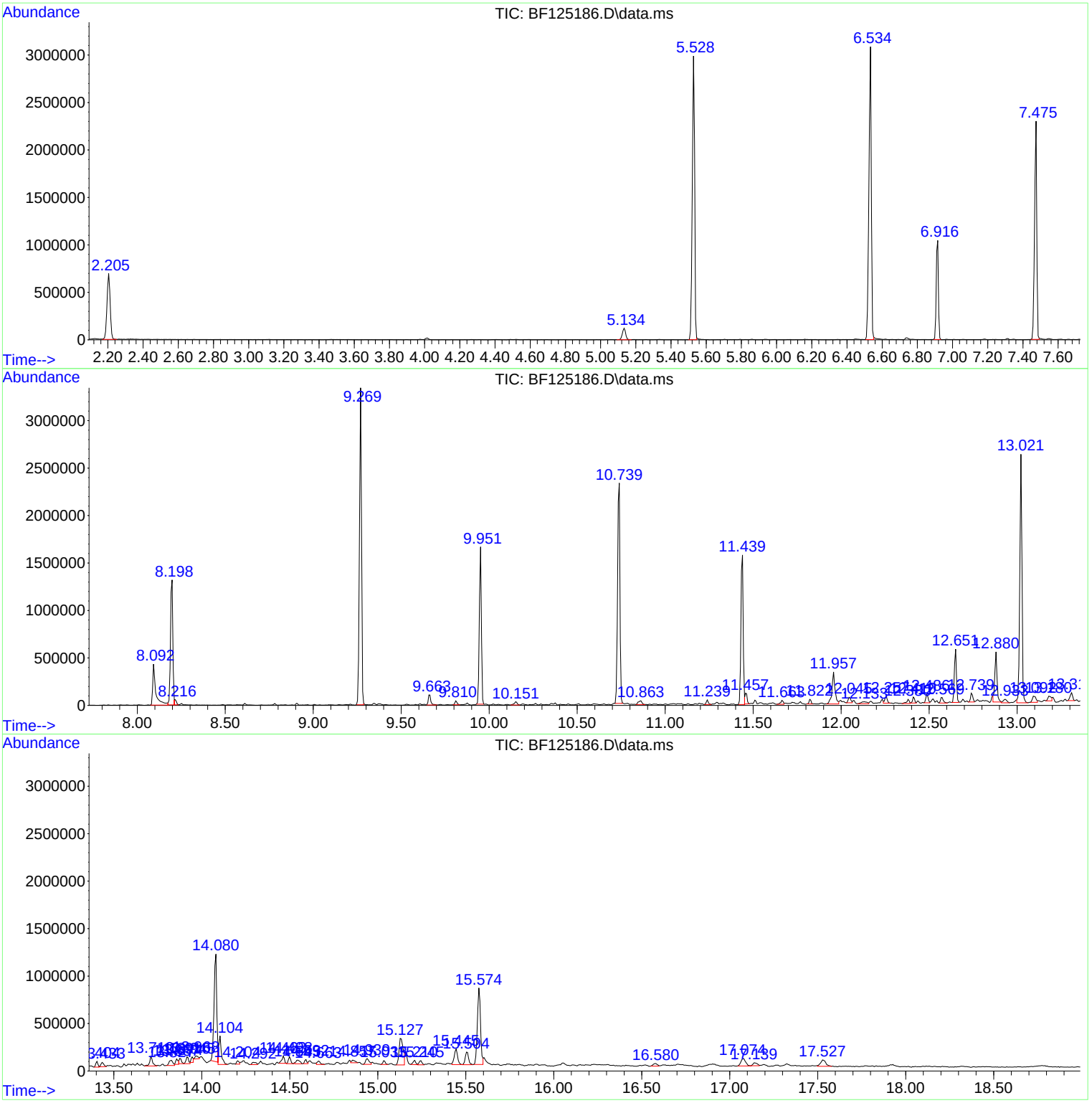
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-4-(177.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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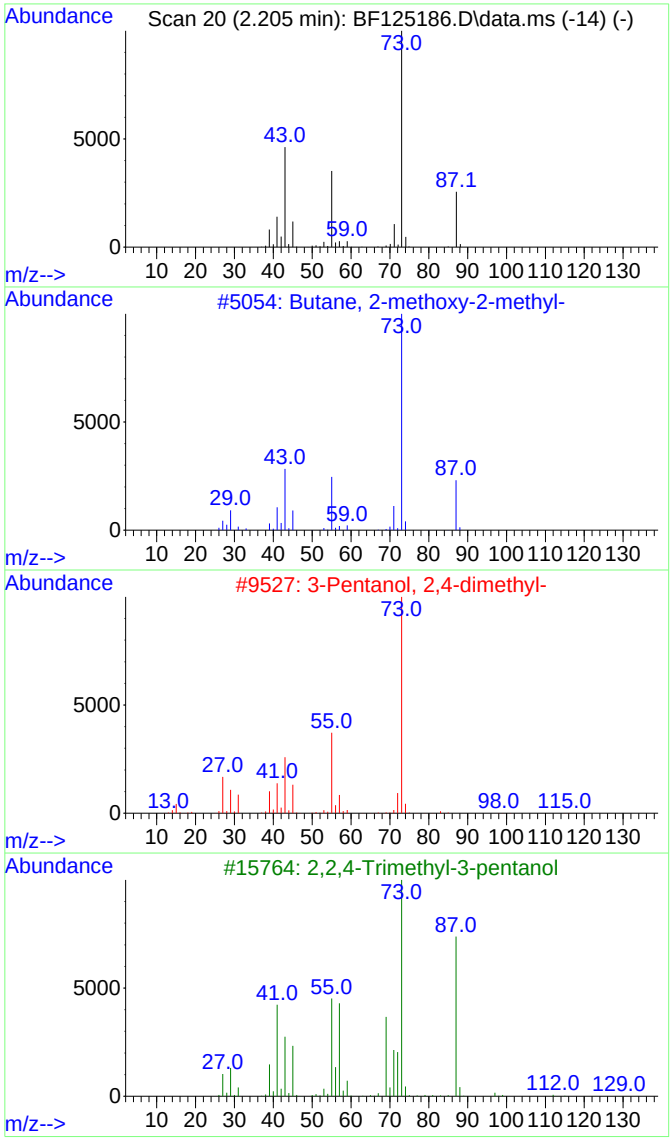
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

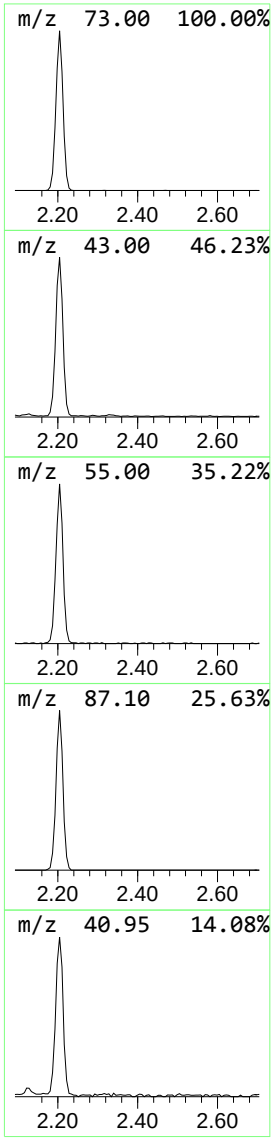
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	19.52 ng	862820	1,4-Dichlorobenzene-d4	6.916

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125186.D
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Operator : JU/CG
Sample : M3467-17
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Instrument :
BNA_F
ClientSampleId :
SAMPLE-4-(177.00)

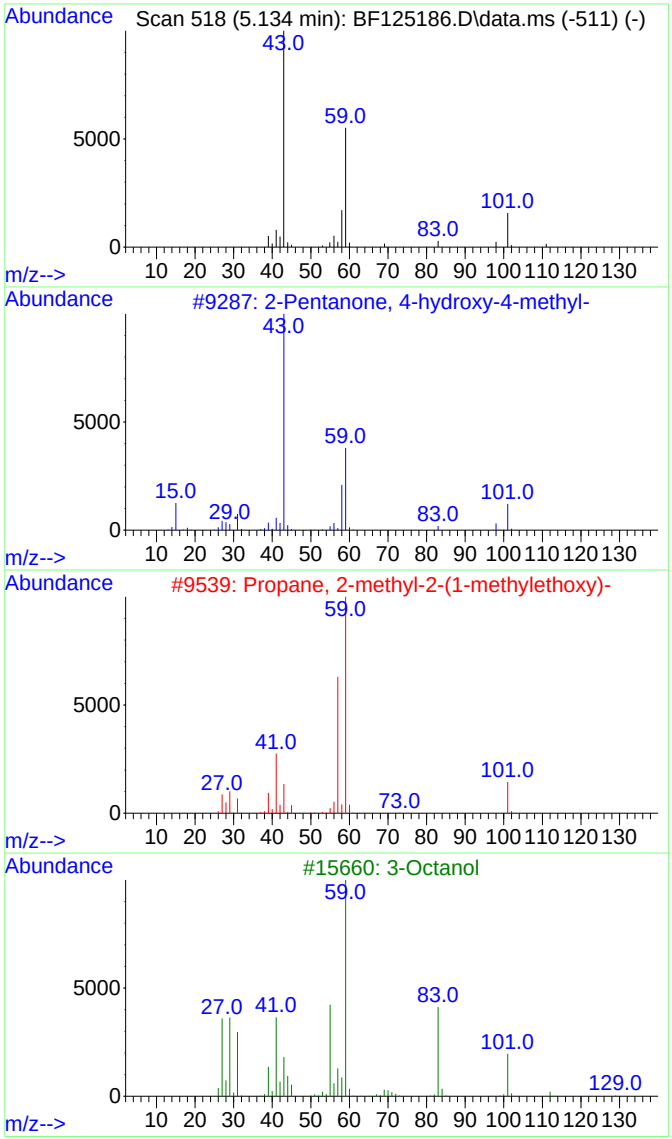
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

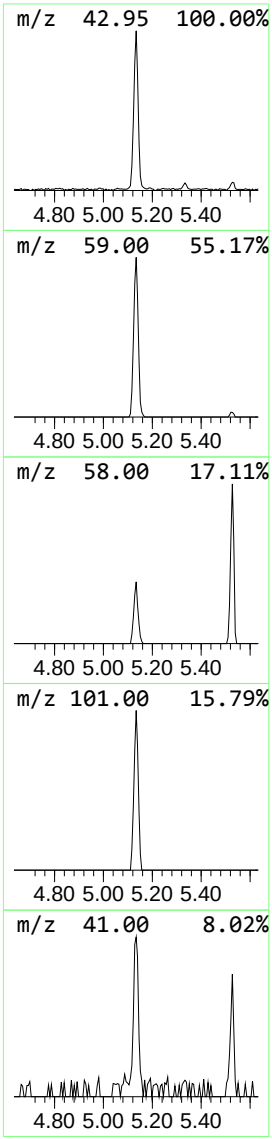
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	3.52 ng	155630	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Octanol	130	C8H18O	000589-98-0	33
4	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





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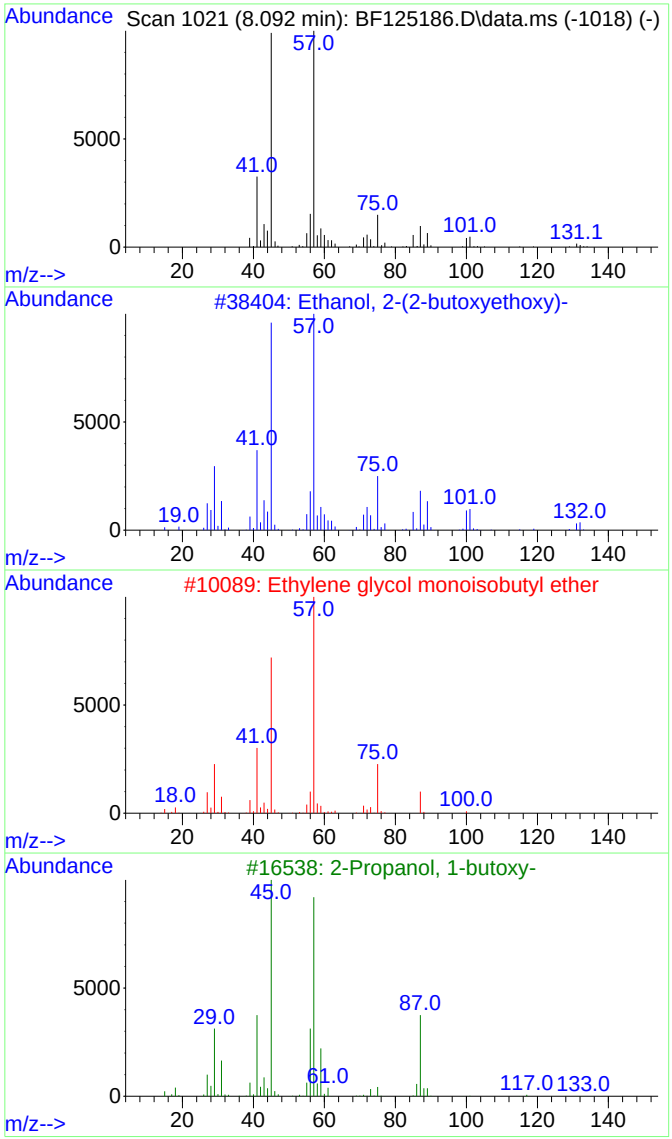
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

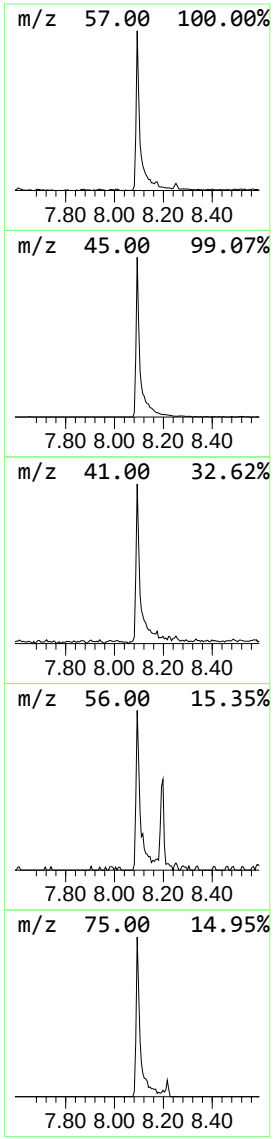
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	8.90 ng	527425	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	59
4	Pentaethylene glycol	238	C10H22O6	004792-15-8	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





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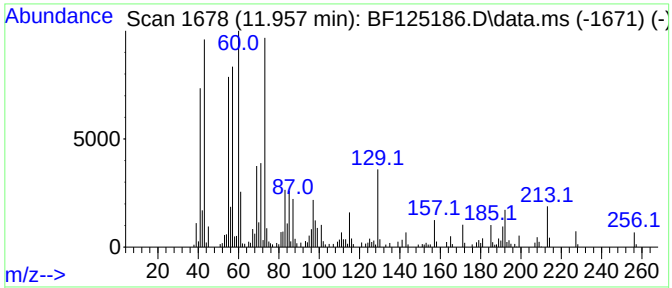
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

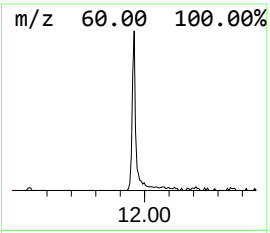
****

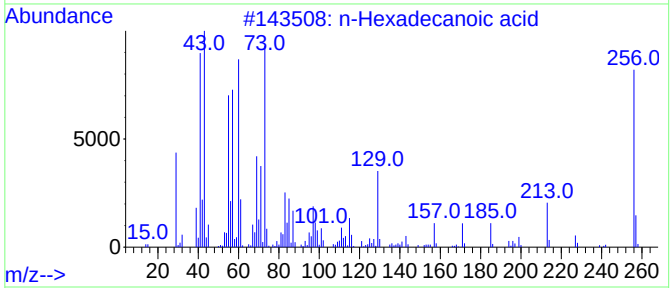
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

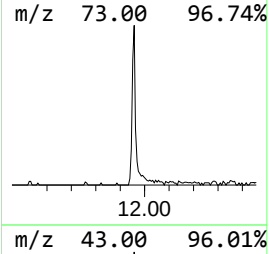
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	5.78 ng	406544	Phenanthrene-d10	11.439

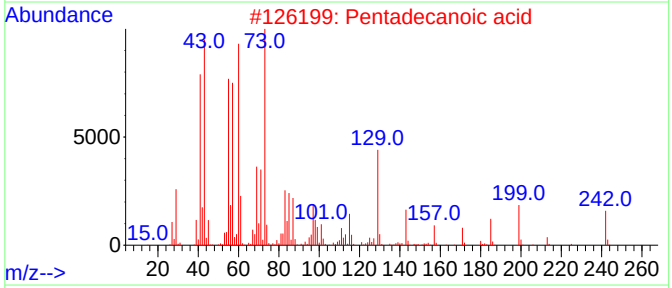
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76

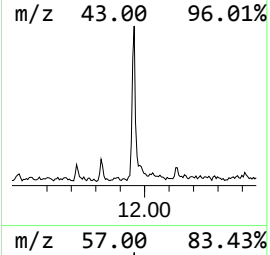


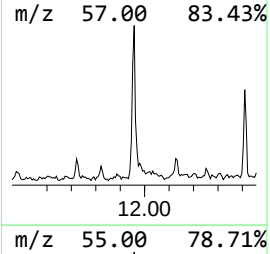


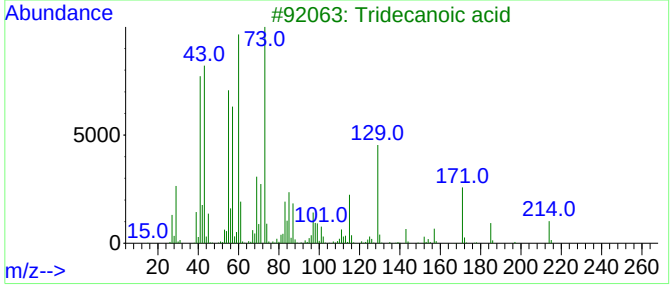


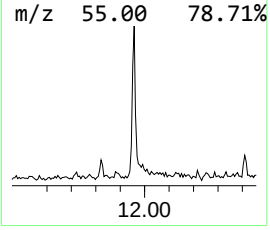












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Instrument :
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ClientSampleId :
SAMPLE-4-(177.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

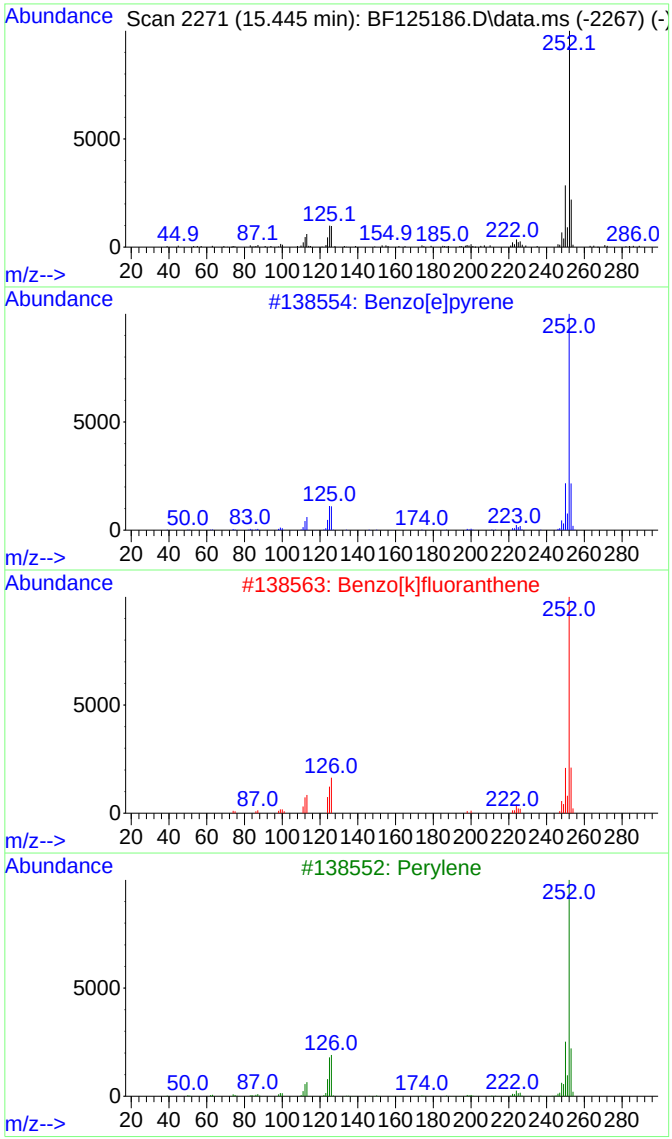
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

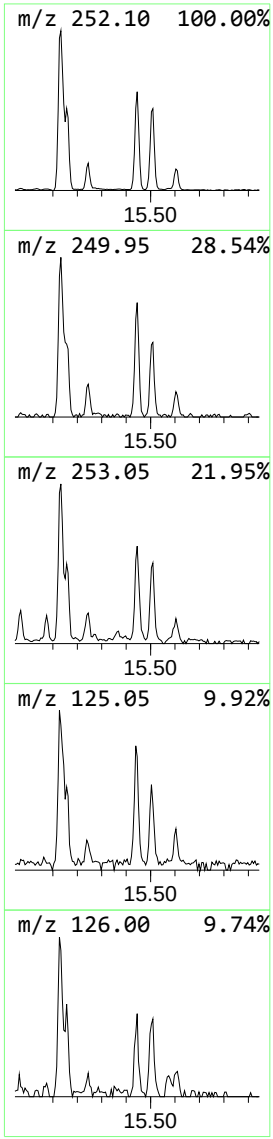
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	4.14 ng	209806	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Perylene	252	C20H12	000198-55-0	90
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082421\
Data File : BF125186.D
Acq On : 24 Aug 2021 15:38
Operator : JU/CG
Sample : M3467-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-4-(177.00)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.205	19.5	ng	862820	1	6.916	884241	20.0
2-Pentanone, 4-...	5.134	3.5	ng	155630	1	6.916	884241	20.0
Ethanol, 2-(2-b...	8.092	8.9	ng	527425	2	8.198	1184760	20.0
n-Hexadecanoic ...	11.957	5.8	ng	406544	4	11.439	1406180	20.0
Benzo[e]pyrene	15.445	4.1	ng	209806	6	15.574	1014250	20.0