LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133874.D
Acq On : 21 Jun 2023 16:52
Operator : CG\JU
Sample : 03296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSIT-R-02

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133874.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	308267	391356	22.06%	2.375%
2	2.251	24	28	37	rVB2	17966	34069	1.92%	0.207%
3	4.481	402	407	412	rBV	16342	20864	1.18%	0.127%
4	5.092	506	511	521	rBV	641763	735191	41.44%	4.462%
5	5.492	575	579	592	rVB	1787348	1580155	89.06%	9.591%
6	5.881	642	645	652	rBV	43554	37837	2.13%	0.230%
7	6.492	745	749	752	rBV	1795761	1582176	89.18%	9.603%
8	6.857	808	811	815	rBV	834322	716865	40.41%	4.351%
9	7.422	902	907	910	rBV	1095700	1030772	58.10%	6.256%
10	8.139	1025	1029	1032	rBV	1068482	847312	47.76%	5.143%
11	9.216	1208	1212	1215	rBV	2190079	1774171	100.00%	10.768%
12	9.898	1324	1328	1331	rBV	898852	758431	42.75%	4.603%
13	10.610	1445	1449	1458	rBV	92380	77428	4.36%	0.470%
14	10.686	1458	1462	1472	rBV	1007401	839125	47.30%	5.093%
15	10.810	1478	1483	1487	rVB3	16279	24704	1.39%	0.150%
16	11.386	1578	1581	1584	rBV	718008	685931	38.66%	4.163%
17	11.410	1584	1585	1589	rVV	174229	131242	7.40%	0.797%
18	11.463	1591	1594	1598	rVB	37211	35818	2.02%	0.217%
19	11.627	1616	1622	1627	rBV2	17410	29416	1.66%	0.179%
20	11.892	1663	1667	1669	rBV	28835	28898	1.63%	0.175%
21	11.915	1669	1671	1676	rVV2	149044	160803	9.06%	0.976%
22	12.004	1683	1686	1689	rBV2	42071	49608	2.80%	0.301%
23	12.192	1714	1718	1720	rBV	24625	25669	1.45%	0.156%
24	12.215	1720	1722	1725	rVB2	26075	25326	1.43%	0.154%
25	12.445	1758	1761	1764	rBV	21972	26578	1.50%	0.161%
26	12.533	1773	1776	1783	rBV	26943	31427	1.77%	0.191%
27	12.610	1783	1789	1793	rBV	438798	394168	22.22%	2.392%
28	12.710	1803	1806	1810	rBV3	44208	55277	3.12%	0.335%
29	12.839	1822	1828	1834	rBV	389615	403030	22.72%	2.446%
30	12.892	1834	1837	1843	rVB3	18684	26336	1.48%	0.160%
31	12.986	1849	1853	1856	rBV	1713241	1404935	79.19%	8.527%
32	13.057	1861	1865	1869	rBV4	32225	54419	3.07%	0.330%
33	13.145	1877	1880	1881	rBV3	24552	22604	1.27%	0.137%
34	13.168	1882	1884	1887	rVB	50931	45473	2.56%	0.276%
35	13.239	1894	1896	1898	rVB	33435	26168	1.47%	0.159%
36	13.274	1898	1902	1905	rBV2	41547	46755	2.64%	0.284%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133874.D
Acq On : 21 Jun 2023 16:52
Operator : CG\JU
Sample : 03296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-02

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.398	1921	1923	1926	rBV2	27891	25147	1.42%	0.153%
38	13.562	1949	1951	1954	rBV3	19996	24967	1.41%	0.152%
39	13.680	1969	1971	1975	rVB	47122	44179	2.49%	0.268%
40	13.792	1988	1990	1993	rVB3	32052	30053	1.69%	0.182%
41	13.821	1993	1995	1997	rBV	32048	26198	1.48%	0.159%
42	13.892	2004	2007	2014	rBV2	120356	156434	8.82%	0.949%
43	14.045	2028	2033	2036	rBV2	763257	898098	50.62%	5.451%
44	14.074	2036	2038	2040	rVB	173706	136110	7.67%	0.826%
45	14.151	2049	2051	2054	rVB2	42840	35019	1.97%	0.213%
46	15.109	2210	2214	2217	rBV	149323	226128	12.75%	1.372%
47	15.421	2265	2267	2274	rVB	79855	102520	5.78%	0.622%
48	15.486	2275	2278	2285	rVB	122942	155525	8.77%	0.944%
49	15.556	2285	2290	2294	rBV	363901	455414	25.67%	2.764%

Sum of corrected areas: 16476129

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Misc :
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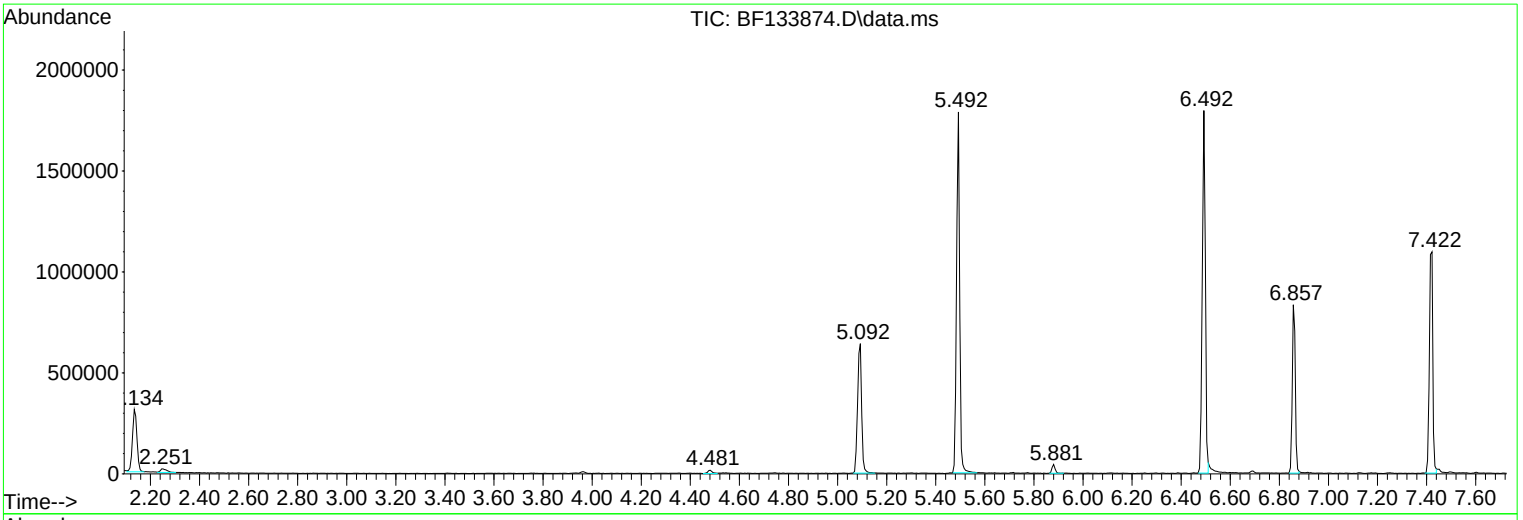
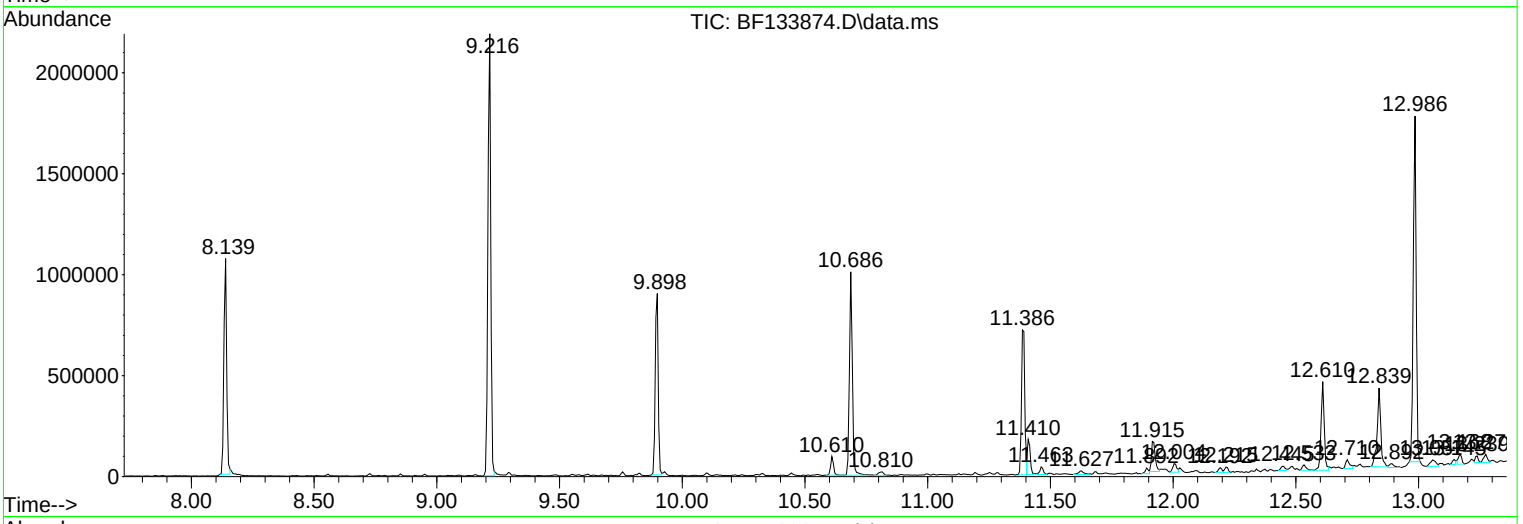
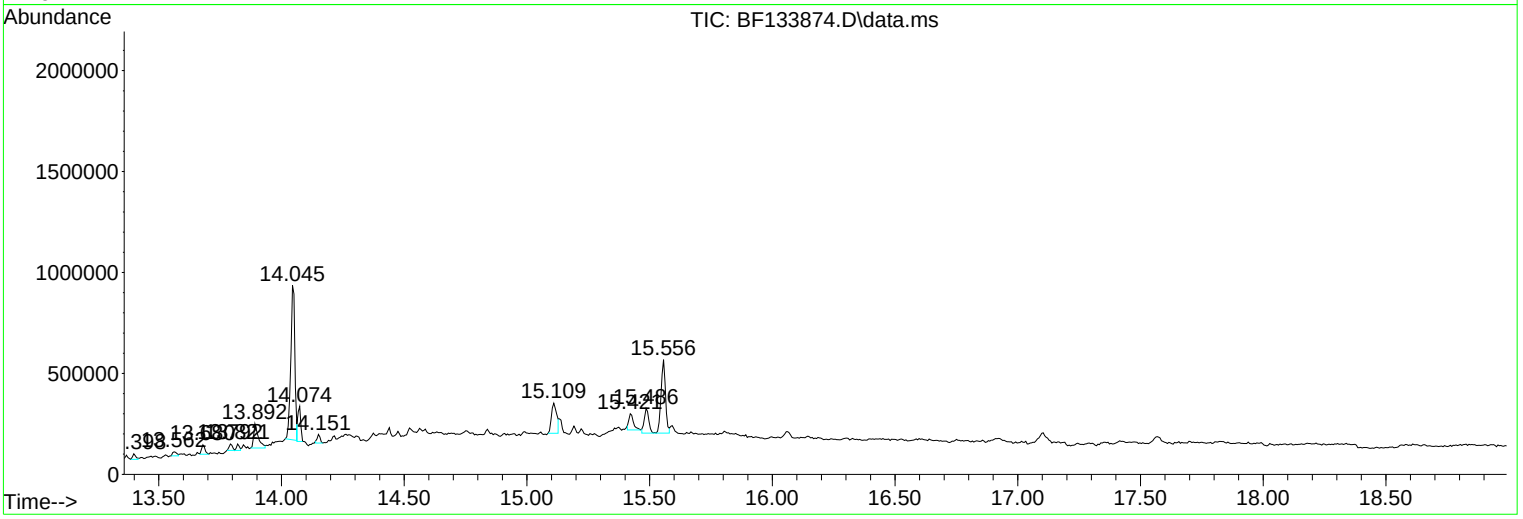
Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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\BF062123\
Data File : BF133874.D
Acq On : 21 Jun 2023 16:52
Operator : CG\JU
Sample : 03296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

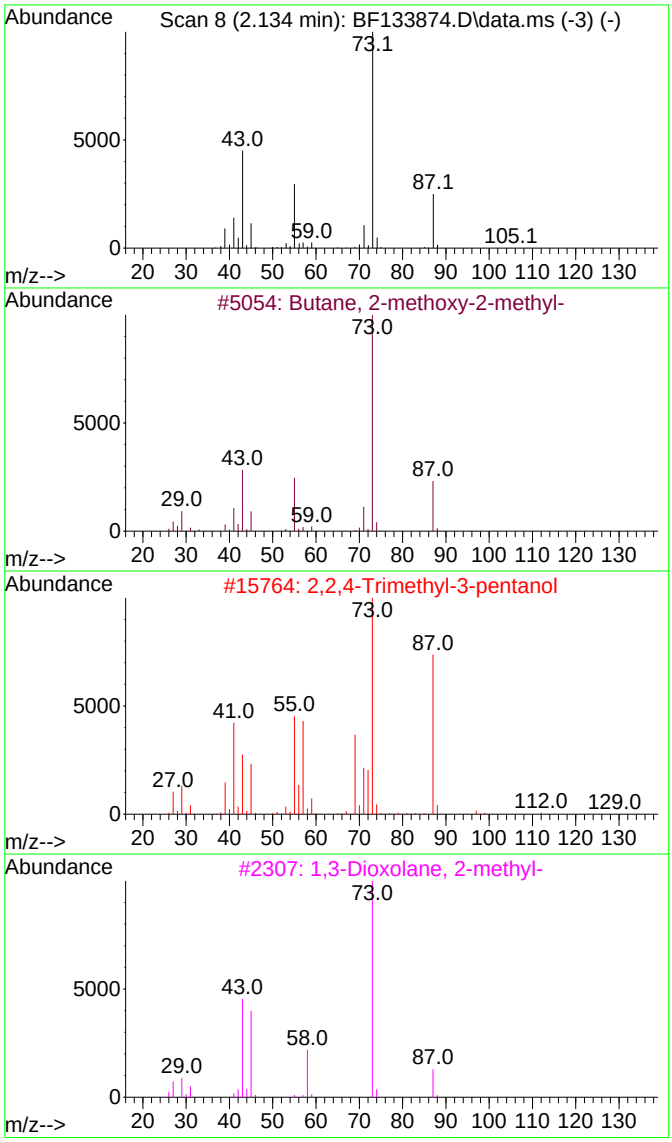
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

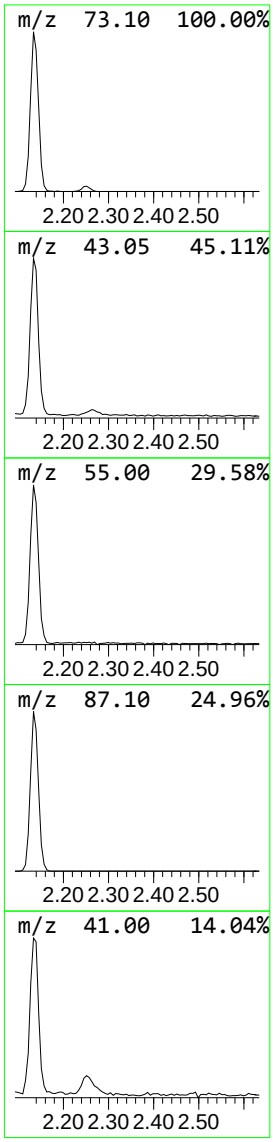
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	10.92 ng	391356	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	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133874.D
Acq On : 21 Jun 2023 16:52
Operator : CG\JU
Sample : 03296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-02

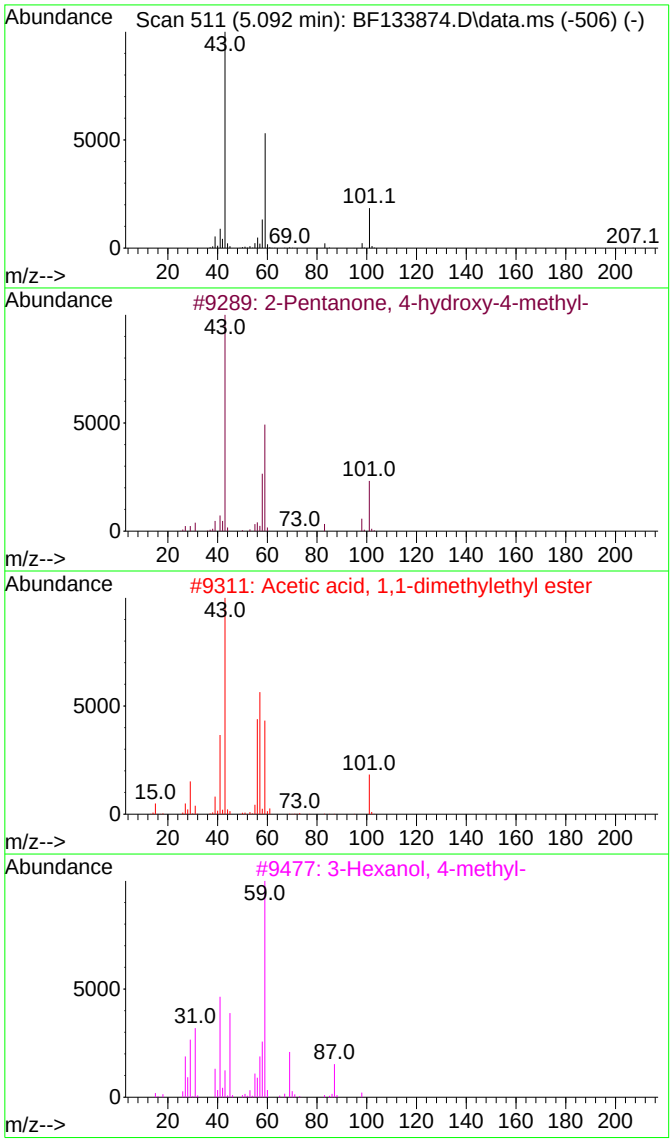
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

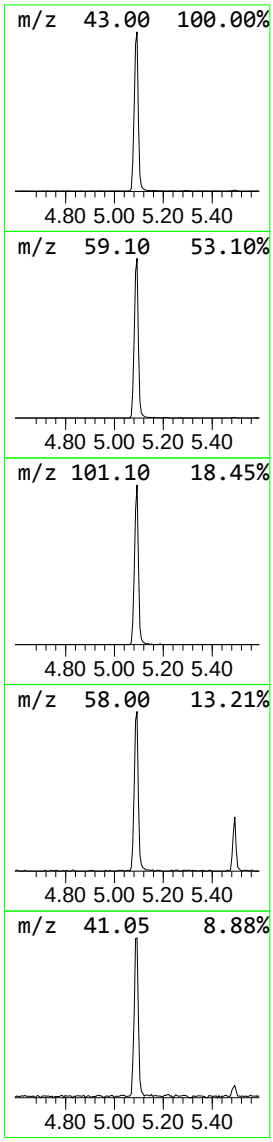
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	20.51 ng	735191	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133874.D
Acq On : 21 Jun 2023 16:52
Operator : CG\JU
Sample : 03296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

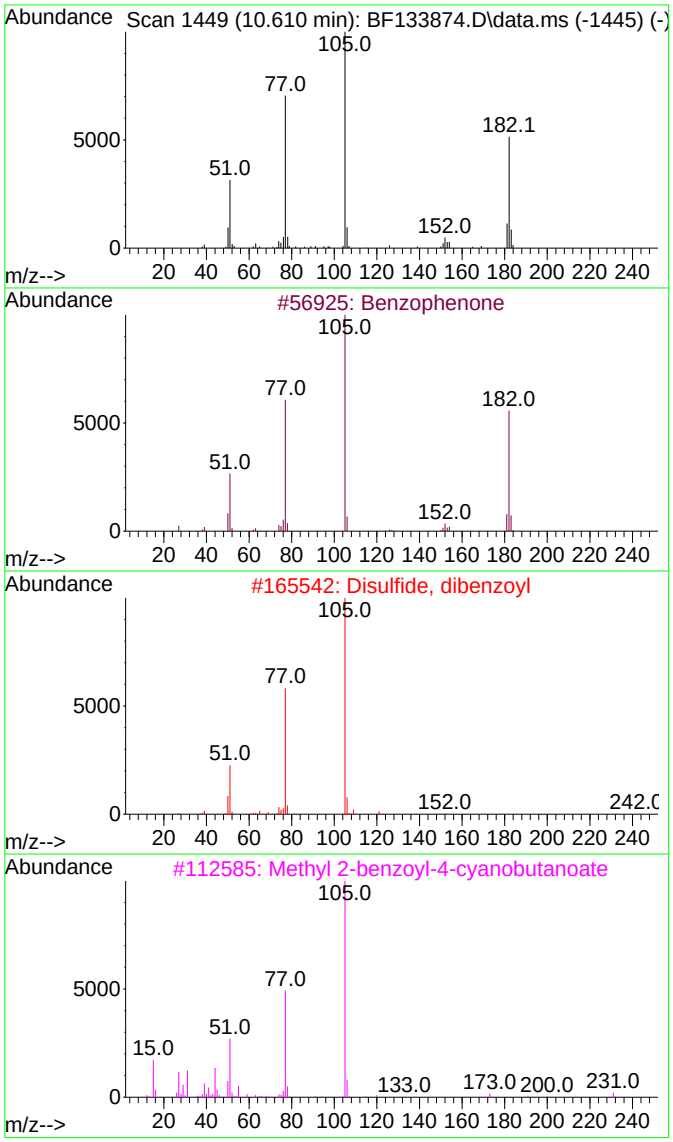
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

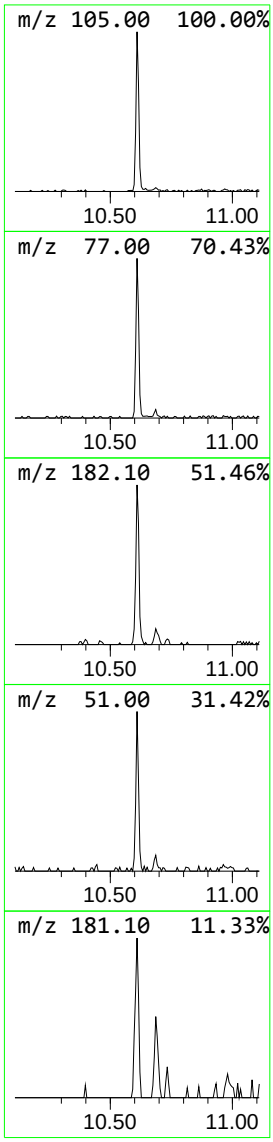
****

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	2.04 ng	77428	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	49
3	Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133874.D
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Operator : CG\JU
Sample : 03296-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

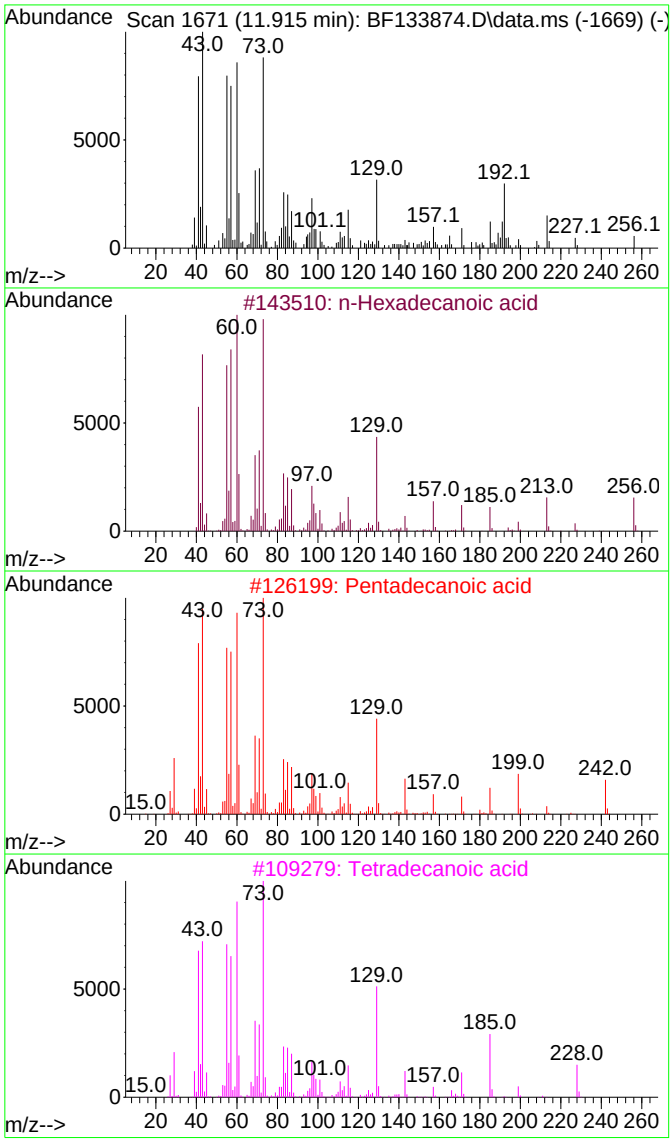
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

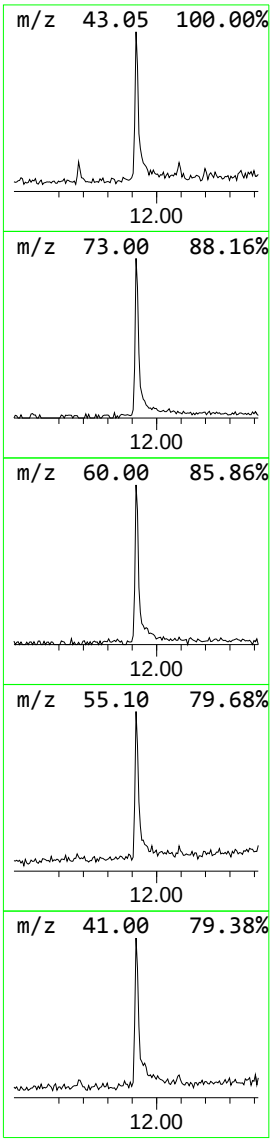
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	4.69 ng	160803	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

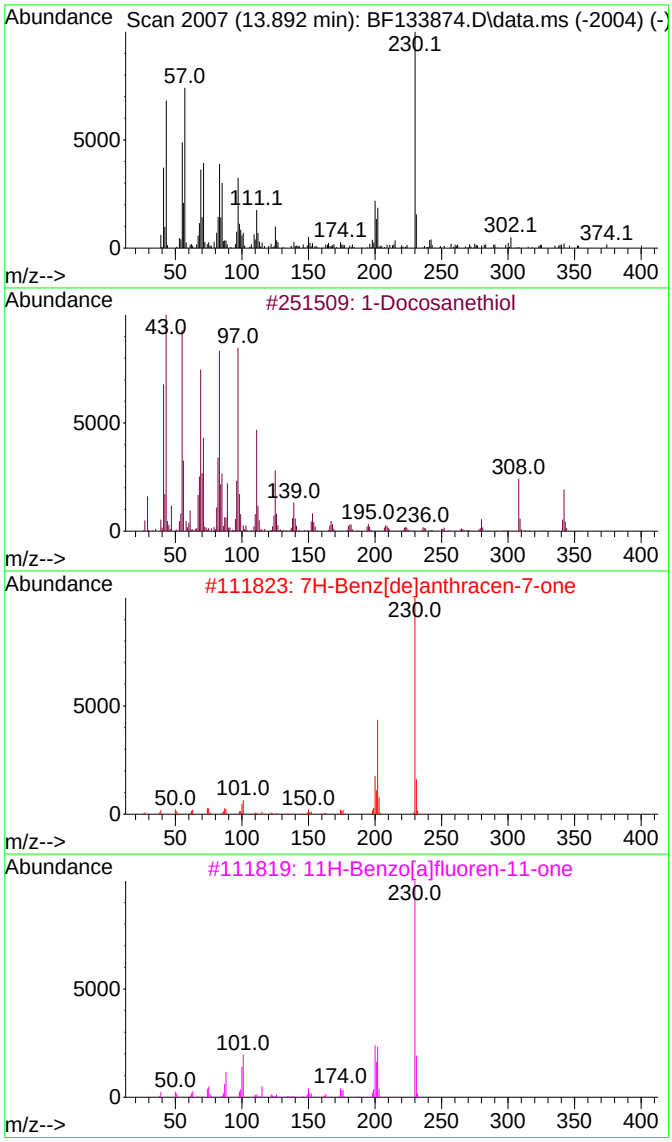
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

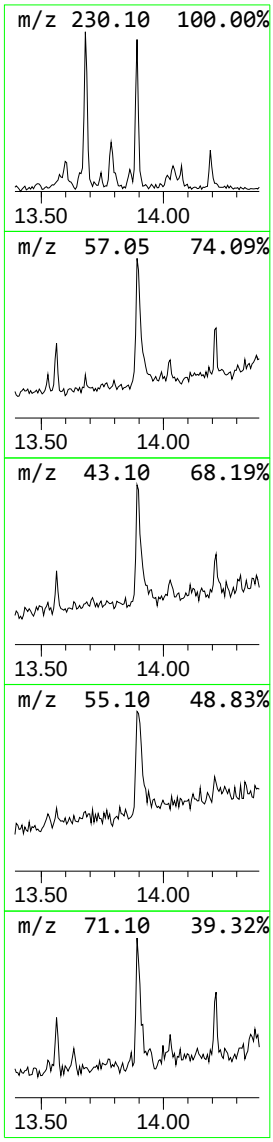
****

Peak Number 5 unknown13.892 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.48 ng	156434	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanethiol	342	C22H46S	007773-83-3	47
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	46
3	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	43
4	Propionic acid, 3-iodo-, hexadec...	424	C19H37IO2	1000406-24-7	38
5	Propionic acid, 3-iodo-, octadec...	452	C21H41IO2	1000406-24-9	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

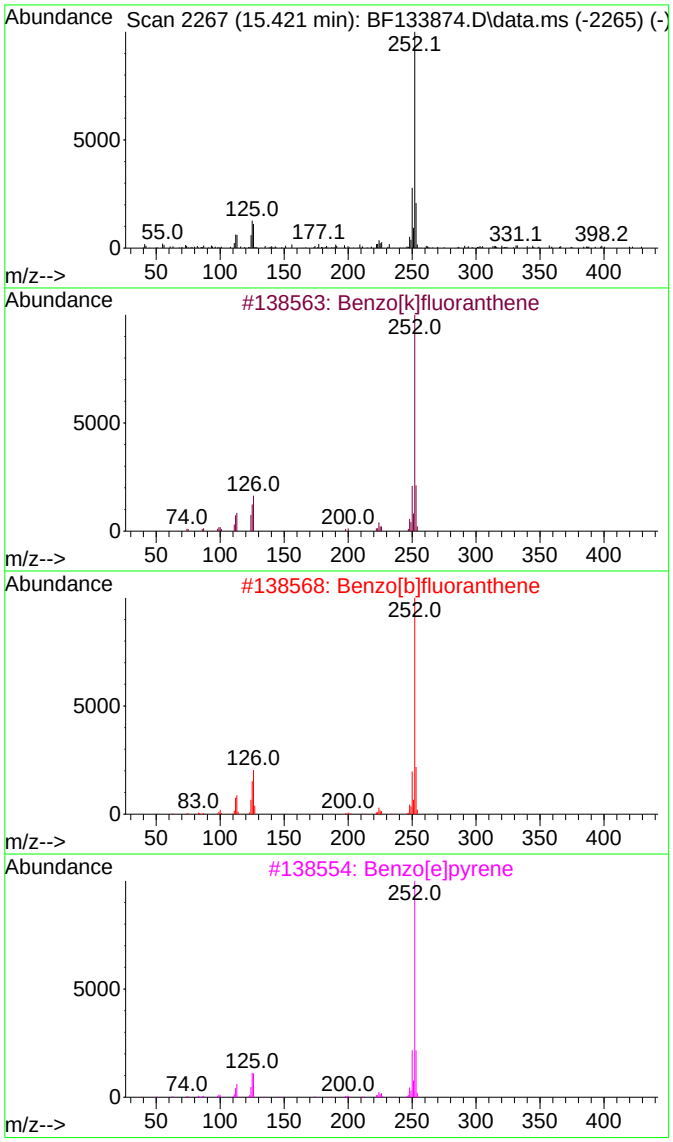
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

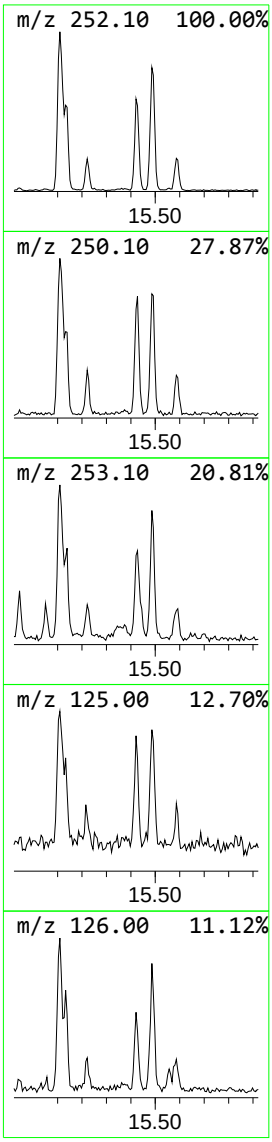
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.421	4.50 ng	102520	Perylene-d12	15.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
3	Benzo[e]pyrene	252	C20H12	000192-97-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Perylene	252	C20H12	000198-55-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133874.D
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Operator : CG\JU
Sample : 03296-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
COMPOSIT-R-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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	10.9	ng	391356	1	6.857	716865	20.0
2-Pentanone, 4-...	5.092	20.5	ng	735191	1	6.857	716865	20.0
Benzophenone	10.610	2.0	ng	77428	3	9.898	758431	20.0
n-Hexadecanoic ...	11.916	4.7	ng	160803	4	11.392	685931	20.0
unknown13.892	13.892	3.5	ng	156434	5	14.051	898098	20.0
Benzo[e]pyrene	15.421	4.5	ng	102520	6	15.556	455414	20.0