LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133822.D
Acq On : 16 Jun 2023 23:37
Operator : CG\JU
Sample : 03223-07 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-05

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: BF133822.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	13	rVB	131913	167117	15.87%	1.527%
2	5.093	507	511	519	rBV	49668	61520	5.84%	0.562%
3	5.493	575	579	596	rVB	967031	902082	85.65%	8.242%
4	6.492	745	749	752	rBV	1037375	872825	82.87%	7.974%
5	6.863	809	812	816	rBV	582229	472707	44.88%	4.319%
6	7.422	903	907	910	rBV	718075	545808	51.82%	4.987%
7	8.145	1026	1030	1033	rBV	645923	591516	56.16%	5.404%
8	9.216	1209	1212	1215	rBV	1415600	1053273	100.00%	9.623%
9	9.757	1301	1304	1307	rBV	21756	20923	1.99%	0.191%
10	9.898	1324	1328	1332	rBV	720389	586432	55.68%	5.358%
11	9.933	1332	1334	1338	rVB	26619	22488	2.14%	0.205%
12	10.104	1359	1363	1368	rVB2	17863	18641	1.77%	0.170%
13	10.445	1418	1421	1427	rBV	26299	32425	3.08%	0.296%
14	10.616	1446	1450	1453	rBV	177891	162986	15.47%	1.489%
15	10.686	1459	1462	1470	rVB	679687	629134	59.73%	5.748%
16	10.816	1480	1484	1487	rBV4	14020	17478	1.66%	0.160%
17	10.922	1499	1502	1505	rBV	23278	21064	2.00%	0.192%
18	10.998	1509	1515	1518	rBV6	11557	18289	1.74%	0.167%
19	11.198	1545	1549	1552	rBV2	15950	16644	1.58%	0.152%
20	11.251	1553	1558	1562	rVV7	11417	23656	2.25%	0.216%
21	11.286	1562	1564	1569	rVB2	26425	27591	2.62%	0.252%
22	11.392	1578	1582	1584	rBV	765710	619678	58.83%	5.662%
23	11.416	1584	1586	1589	rVV	373390	285220	27.08%	2.606%
24	11.469	1592	1595	1598	rVB	76503	63169	6.00%	0.577%
25	11.627	1618	1622	1627	rVB2	29907	38912	3.69%	0.356%
26	11.851	1656	1660	1663	rBV6	9996	16158	1.53%	0.148%
27	11.892	1663	1667	1669	rBV2	38909	46949	4.46%	0.429%
28	11.922	1669	1672	1677	rVB2	120372	118640	11.26%	1.084%
29	12.010	1683	1687	1689	rBV	62847	67084	6.37%	0.613%
30	12.033	1689	1691	1695	rVB	30835	29982	2.85%	0.274%
31	12.192	1716	1718	1720	rBV	34220	32179	3.06%	0.294%
32	12.221	1720	1723	1726	rVB	34579	34597	3.28%	0.316%
33	12.451	1759	1762	1765	rBV2	27662	35061	3.33%	0.320%
34	12.533	1774	1776	1779	rBV	26744	29999	2.85%	0.274%
35	12.610	1786	1789	1793	rBV	480396	432022	41.02%	3.947%
36	12.710	1803	1806	1809	rBV2	33596	40312	3.83%	0.368%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133822.D
Acq On : 16 Jun 2023 23:37
Operator : CG\JU
Sample : 03223-07 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-05

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	12.845	1823	1829	1834	rBV	424965	469348	44.56%	4.288%
38	12.986	1847	1853	1861	rBV	1123091	983835	93.41%	8.989%
39	13.174	1883	1885	1888	rVB	57222	48237	4.58%	0.441%
40	13.239	1894	1896	1899	rVB	33460	26330	2.50%	0.241%
41	13.274	1900	1902	1905	rVV2	33422	32978	3.13%	0.301%
42	13.898	2005	2008	2013	rBV2	70642	90871	8.63%	0.830%
43	14.051	2029	2034	2036	rBV2	441482	539143	51.19%	4.926%
44	14.074	2036	2038	2046	rVB	152080	146630	13.92%	1.340%
45	15.115	2212	2215	2223	rVB	132336	254632	24.18%	2.326%
46	15.562	2288	2291	2295	rBV	163574	198672	18.86%	1.815%

Sum of corrected areas: 10945237

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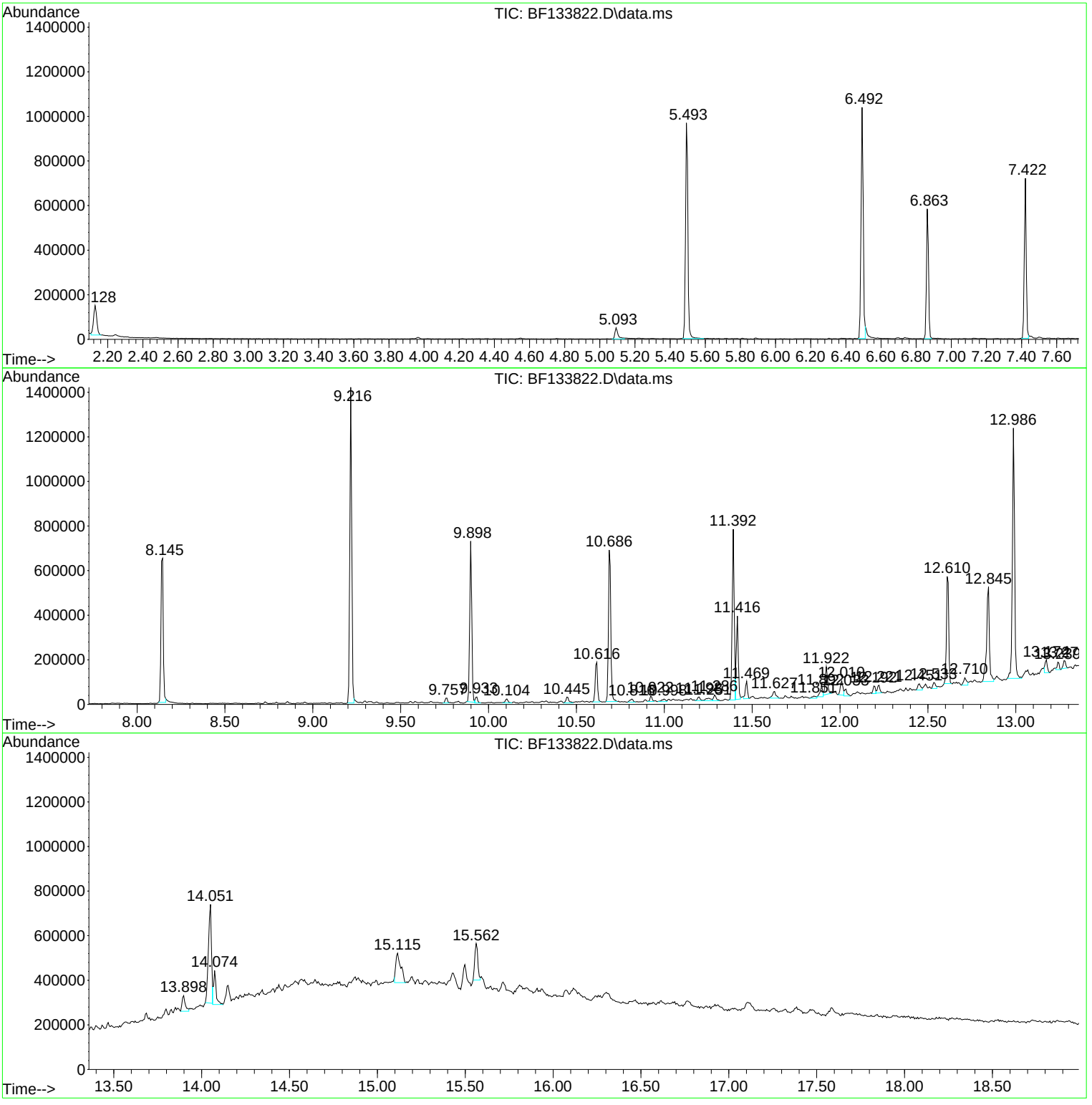
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-05

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\BF061623\
Data File : BF133822.D
Acq On : 16 Jun 2023 23:37
Operator : CG\JU
Sample : 03223-07 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-05

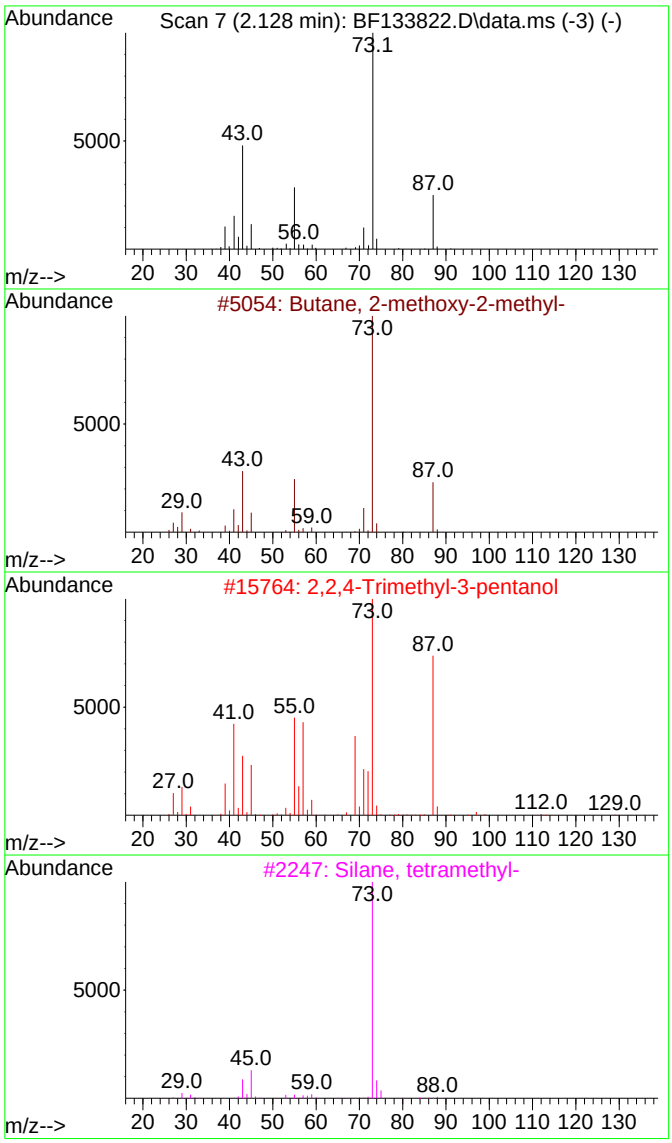
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

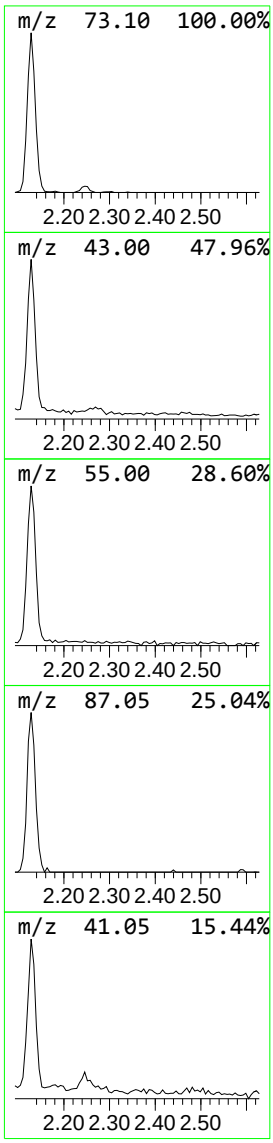
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	7.07 ng	167117	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	16





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Operator : CG\JU
Sample : 03223-07 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-05

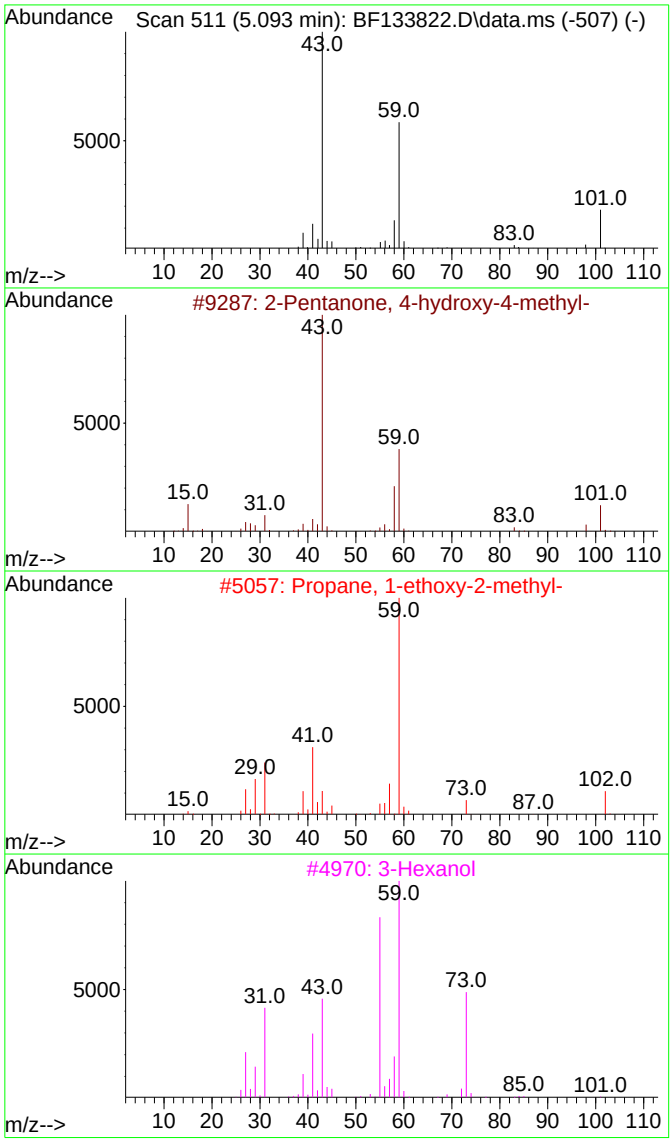
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

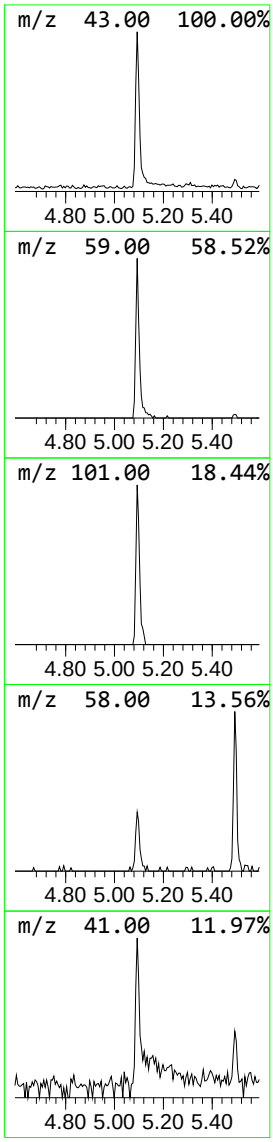
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.60 ng	61520	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	37
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	25
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-05

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

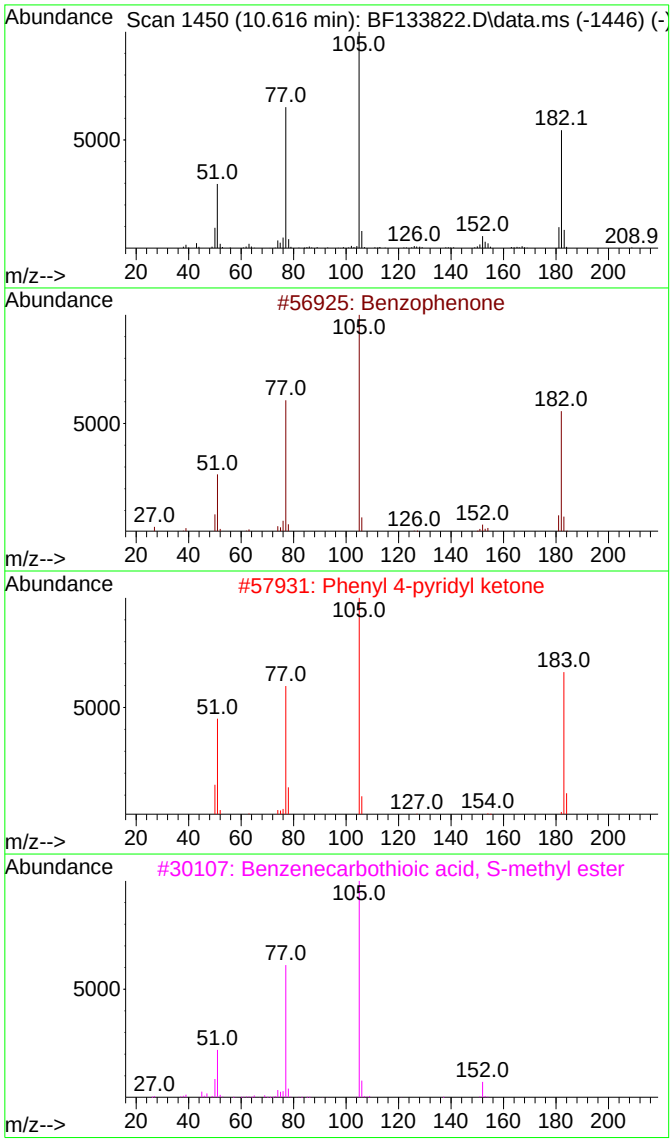
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

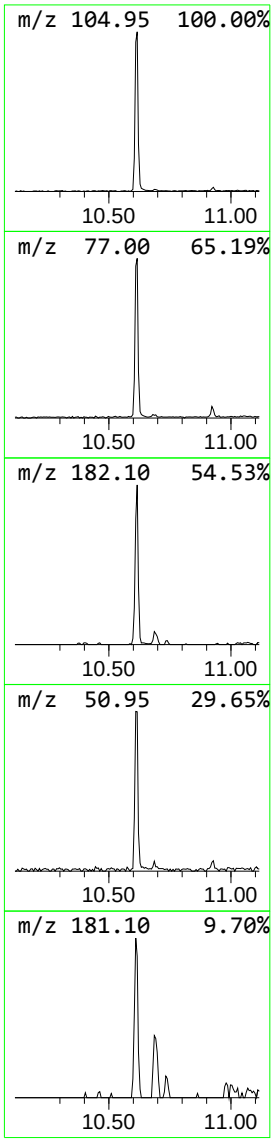
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	5.56 ng	162986	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	58
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	53
5	Benzoic acid, 2-(benzoylthio)thi...	341	C17H11NO3S2	1000258-72-7	47





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Data File : BF133822.D
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-05

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

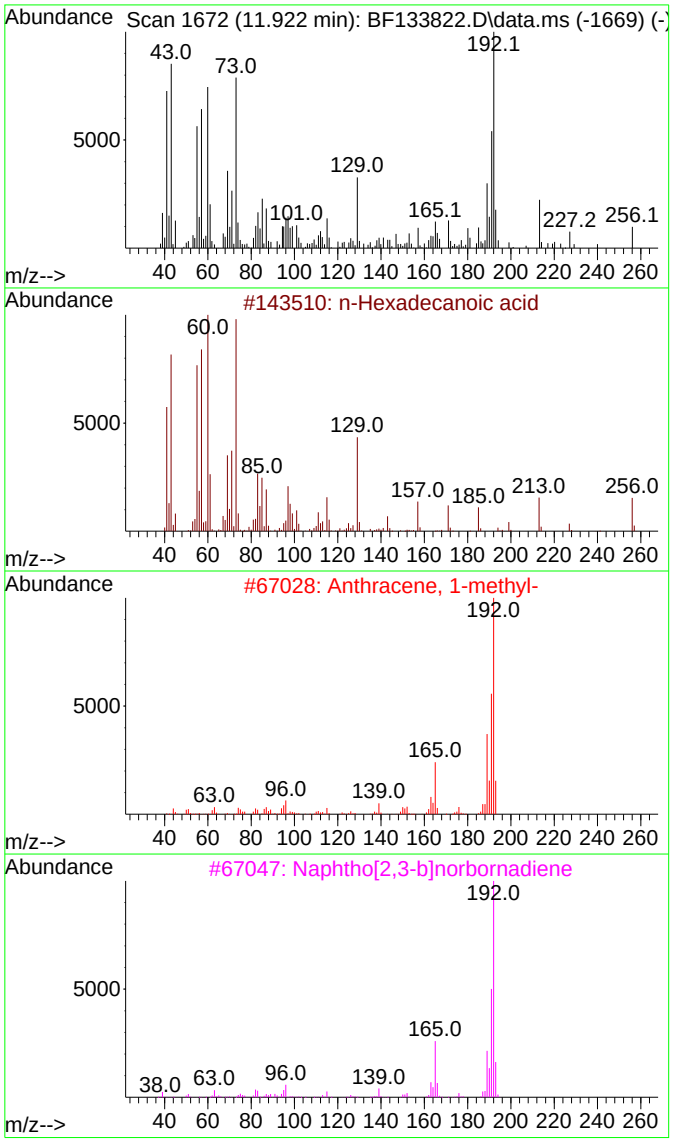
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

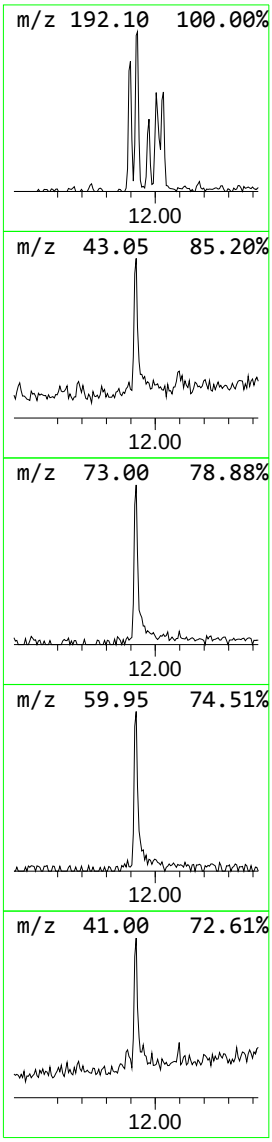
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.83 ng	118640	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	74
3	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	52
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	51
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	51





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Sample : 03223-07 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-05

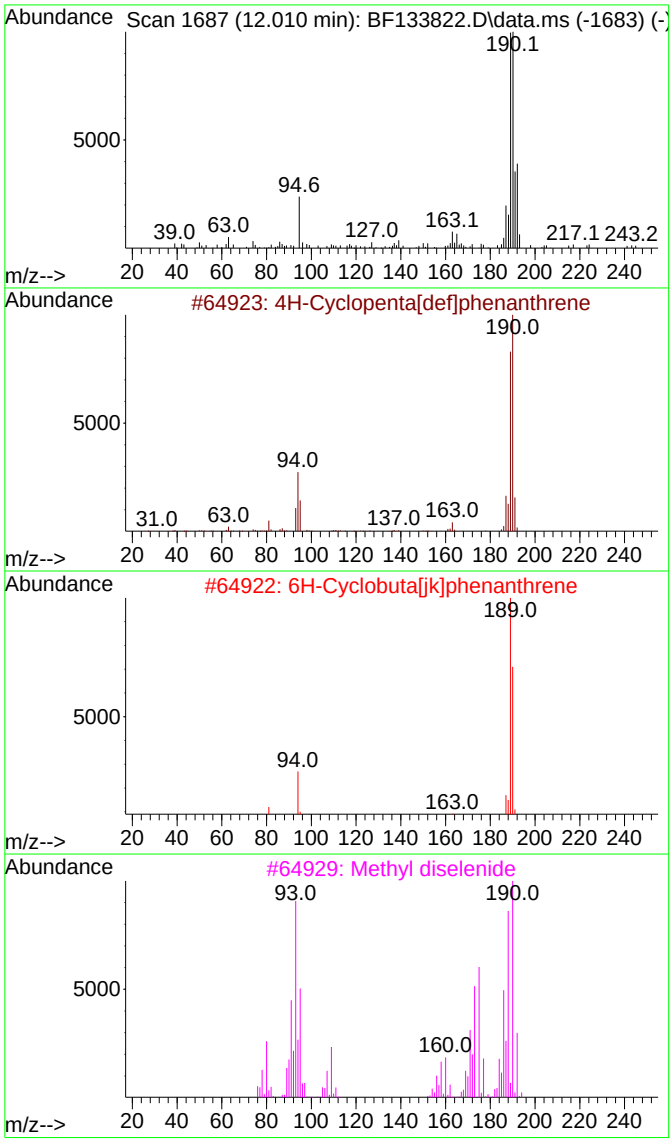
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

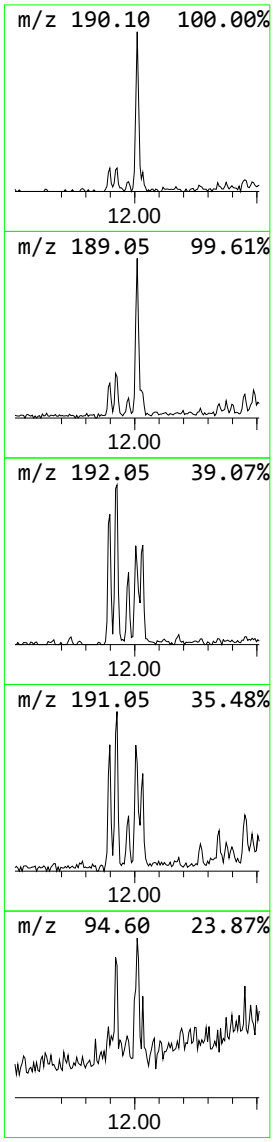
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	2.17 ng	67084	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Methyl diselenide	190	C2H6Se2	007101-31-7	49
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
5	1-Aminocyclopentanecarboxylic ac...	375	C19H34ClNO4	1000329-17-1	25





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-05

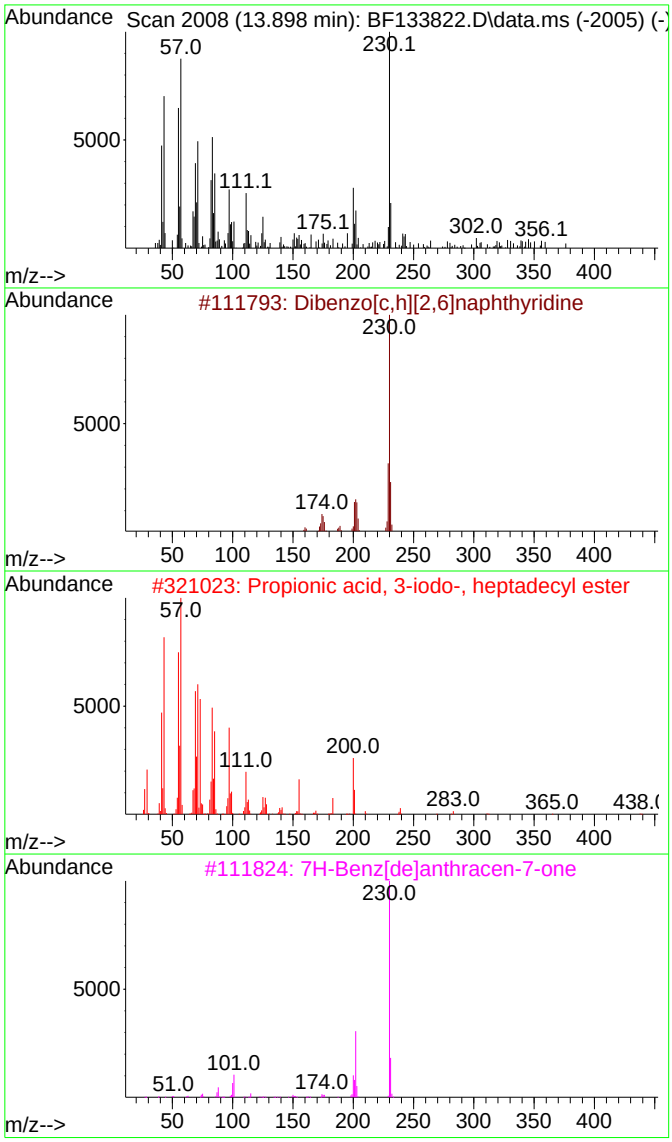
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

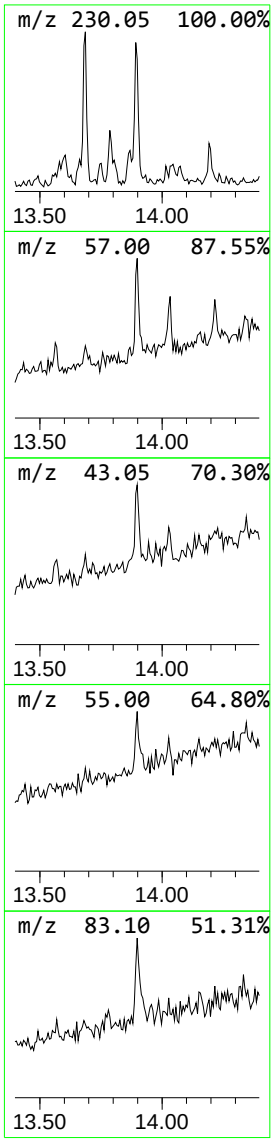
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Dibenzo[c,h][2,6]naphthyridine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	3.37 ng	90871	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[c,h][2,6]naphthyridine	230	C16H10N2	000218-30-4	64
2	Propionic acid, 3-iodo-, heptade...	438	C20H39IO2	1000406-24-8	35
3	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	30
4	o-Terphenyl	230	C18H14	000084-15-1	30
5	p-Terphenyl	230	C18H14	000092-94-4	30





Tentatively Identified Compound (LSC) summary

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Data File : BF133822.D
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-05

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...	2.128	7.1	ng	167117	1	6.863	472707	20.0
2-Pentanone, 4-...	5.093	2.6	ng	61520	1	6.863	472707	20.0
Benzophenone	10.616	5.6	ng	162986	3	9.898	586432	20.0
n-Hexadecanoic ...	11.922	3.8	ng	118640	4	11.392	619678	20.0
4H-Cyclopenta[d...	12.010	2.2	ng	67084	4	11.392	619678	20.0
Dibenzo[c,h][2,...	13.898	3.4	ng	90871	5	14.051	539143	20.0