LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133813.D
Acq On : 16 Jun 2023 18:36
Operator : CG\JU
Sample : 03223-13 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-11

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: BF133813.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	5	9	19	rVB2	67259	104630	8.01%	0.843%
2	5.093	507	511	519	rVB	48487	54355	4.16%	0.438%
3	5.492	575	579	592	rVB	1213527	1063055	81.41%	8.569%
4	6.492	745	749	752	rBV	1263925	1033002	79.11%	8.327%
5	6.863	809	812	818	rBV	711041	540392	41.38%	4.356%
6	7.422	903	907	910	rBV	860874	686132	52.55%	5.531%
7	8.139	1026	1029	1033	rBV	778156	683156	52.32%	5.507%
8	9.216	1208	1212	1215	rBV	1690408	1305779	100.00%	10.526%
9	9.898	1324	1328	1331	rBV	879277	692196	53.01%	5.580%
10	9.927	1331	1333	1337	rVB	29743	26627	2.04%	0.215%
11	10.104	1357	1363	1366	rBV2	19776	21749	1.67%	0.175%
12	10.445	1417	1421	1425	rBV2	23697	23929	1.83%	0.193%
13	10.610	1445	1449	1453	rBV	137288	125195	9.59%	1.009%
14	10.686	1458	1462	1479	rVB	832626	746810	57.19%	6.020%
15	10.810	1479	1483	1487	rBV4	15282	22865	1.75%	0.184%
16	10.922	1499	1502	1509	rVB3	17914	18866	1.44%	0.152%
17	11.286	1562	1564	1570	rVB	17983	16399	1.26%	0.132%
18	11.392	1578	1582	1584	rBV	803772	692742	53.05%	5.584%
19	11.416	1584	1586	1589	rVV	227573	185644	14.22%	1.496%
20	11.463	1589	1594	1597	rVB	47077	50927	3.90%	0.411%
21	11.622	1616	1621	1629	rBV2	27872	42094	3.22%	0.339%
22	11.892	1664	1667	1669	rBV	34645	36054	2.76%	0.291%
23	11.921	1669	1672	1676	rVV2	101288	119305	9.14%	0.962%
24	11.969	1676	1680	1683	rVV2	21984	34774	2.66%	0.280%
25	12.004	1683	1686	1689	rVV	58985	68174	5.22%	0.550%
26	12.027	1689	1690	1695	rVB	26358	22751	1.74%	0.183%
27	12.192	1715	1718	1720	rBV	29545	28829	2.21%	0.232%
28	12.216	1720	1722	1726	rVB3	23772	27057	2.07%	0.218%
29	12.445	1758	1761	1765	rBV	33707	43200	3.31%	0.348%
30	12.486	1765	1768	1770	rVV3	26721	25642	1.96%	0.207%
31	12.533	1773	1776	1782	rVB3	28586	32868	2.52%	0.265%
32	12.610	1786	1789	1793	rVB	457563	371040	28.42%	2.991%
33	12.710	1804	1806	1808	rVB3	19891	16694	1.28%	0.135%
34	12.839	1822	1828	1834	rBV	350427	370363	28.36%	2.986%
35	12.898	1834	1838	1841	rVB2	16379	24549	1.88%	0.198%
36	12.986	1849	1853	1860	rVB	1284335	1090357	83.50%	8.789%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133813.D
Acq On : 16 Jun 2023 18:36
Operator : CG\JU
Sample : 03223-13 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-11

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	13.063	1862	1866	1869	rBV4	27518	42610	3.26%	0.343%
38	13.168	1882	1884	1888	rVB	57331	49899	3.82%	0.402%
39	13.239	1893	1896	1898	rVB	31037	25533	1.96%	0.206%
40	13.274	1899	1902	1905	rVV2	39047	41048	3.14%	0.331%
41	13.333	1910	1912	1915	rBV3	18169	19345	1.48%	0.156%
42	13.368	1916	1918	1921	rVV	21517	18442	1.41%	0.149%
43	13.398	1921	1923	1927	rVV2	28618	27170	2.08%	0.219%
44	13.680	1969	1971	1974	rVB	34383	29362	2.25%	0.237%
45	13.898	2005	2008	2014	rVB4	56473	84194	6.45%	0.679%
46	14.045	2028	2033	2036	rBV2	600053	747619	57.25%	6.027%
47	14.074	2036	2038	2046	rVV	177691	154556	11.84%	1.246%
48	14.145	2048	2050	2054	rVB2	65165	74824	5.73%	0.603%
49	15.110	2211	2214	2217	rBV	117703	163068	12.49%	1.315%
50	15.492	2276	2279	2286	rVB	108266	153211	11.73%	1.235%
51	15.557	2286	2290	2294	rBV	245155	326178	24.98%	2.629%

Sum of corrected areas: 12405260

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
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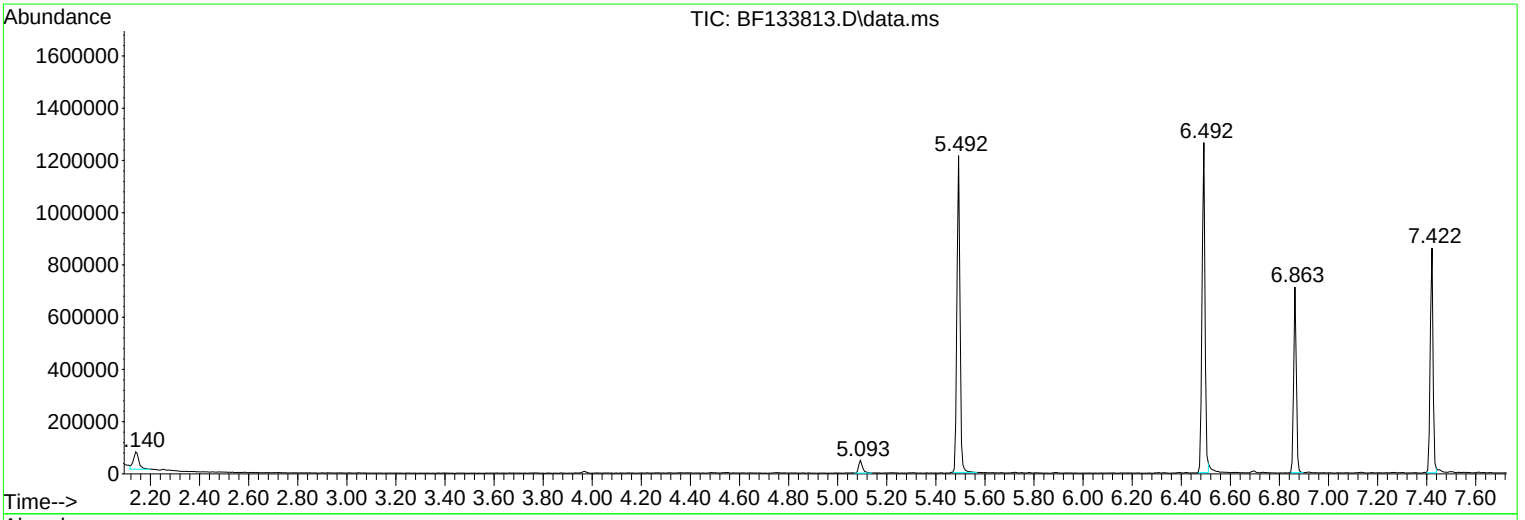
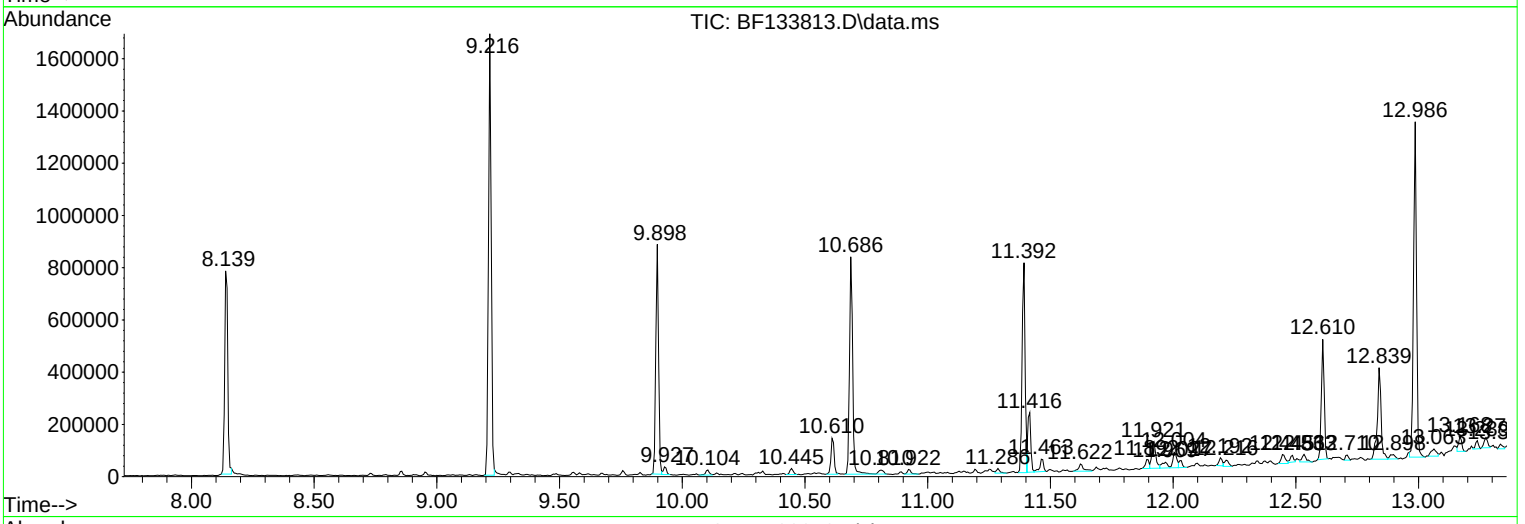
Acq On : 16 Jun 2023 18:36
Operator : CG\JU
Sample : 03223-13 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

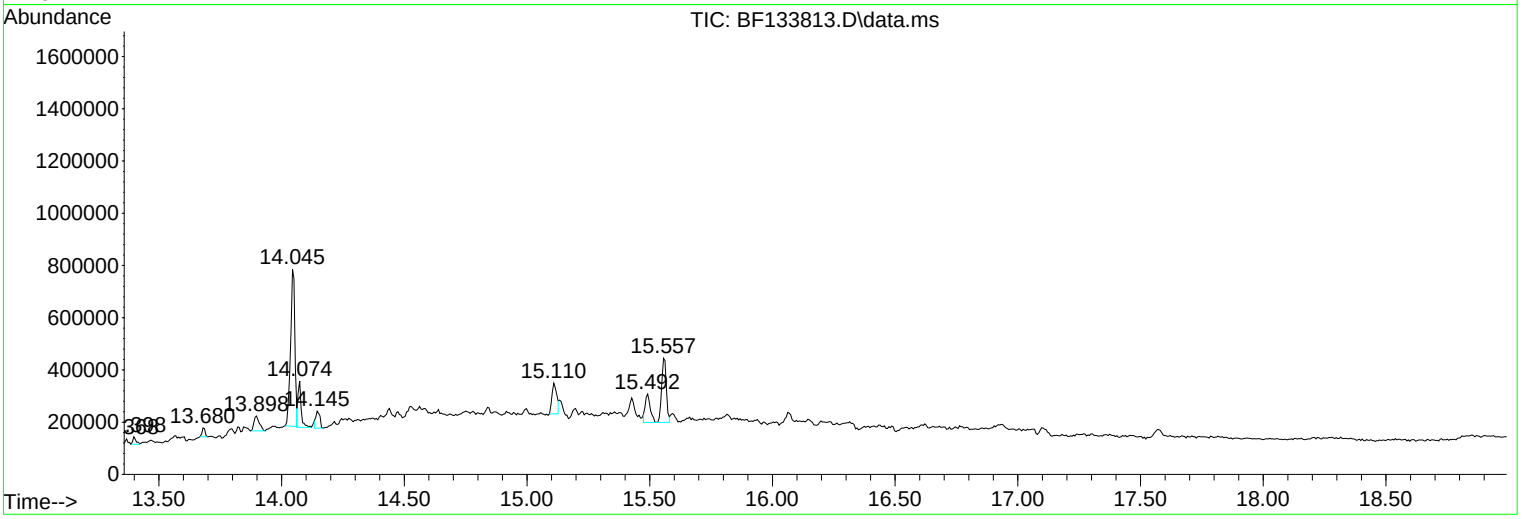
Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-11

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 : BF133813.D
Acq On : 16 Jun 2023 18:36
Operator : CG\JU
Sample : 03223-13 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-11

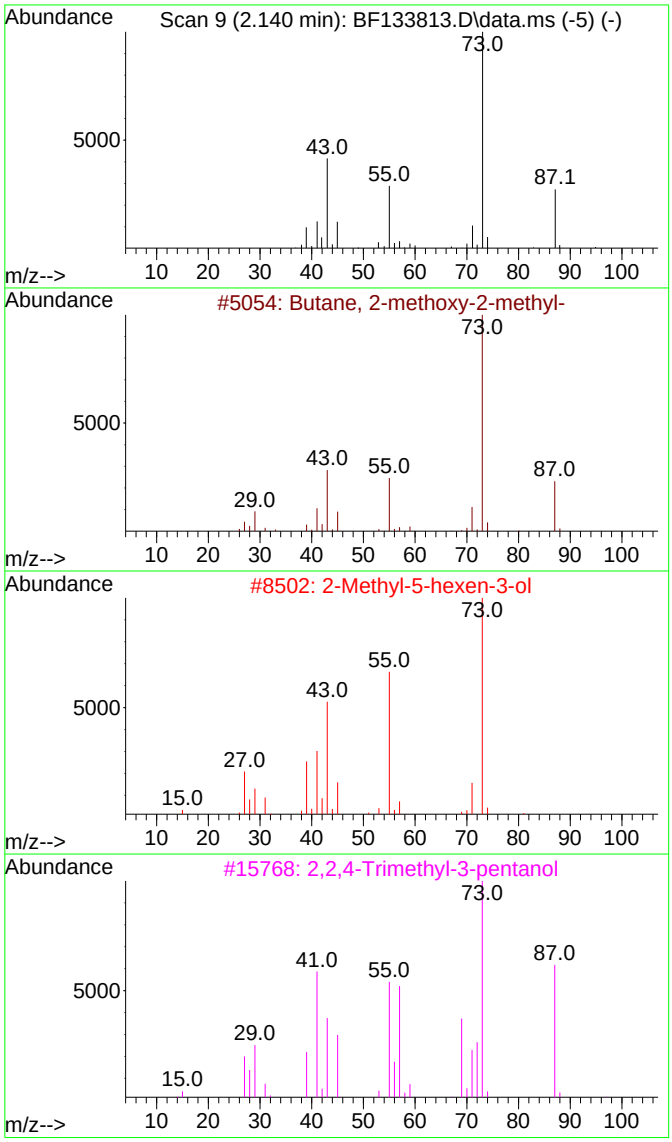
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

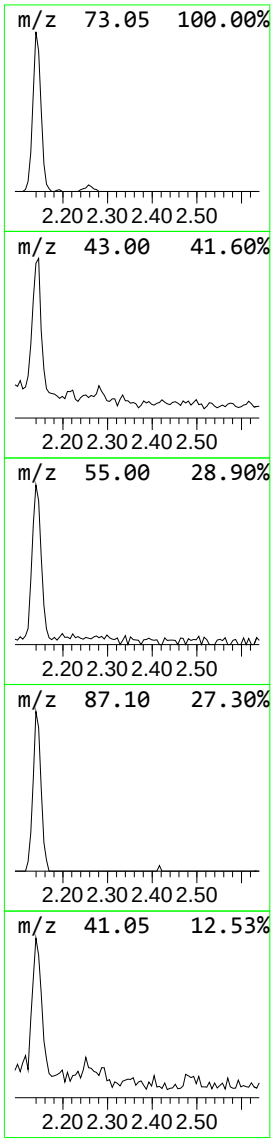
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	3.87 ng	104630	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	83
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	47
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133813.D
Acq On : 16 Jun 2023 18:36
Operator : CG\JU
Sample : 03223-13 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-11

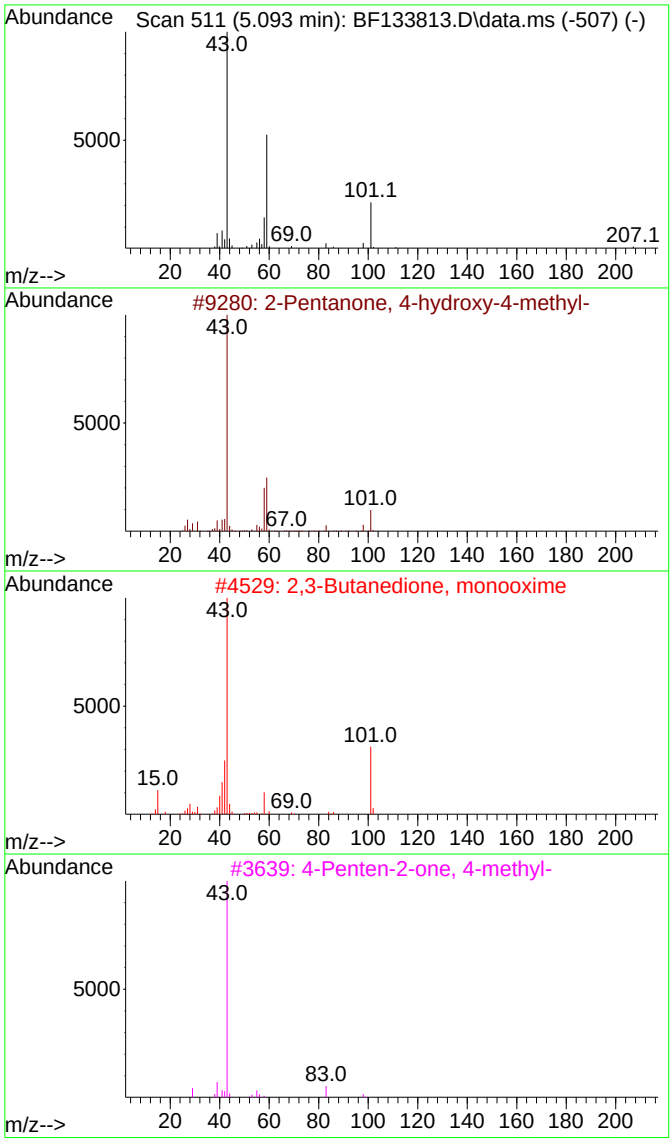
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

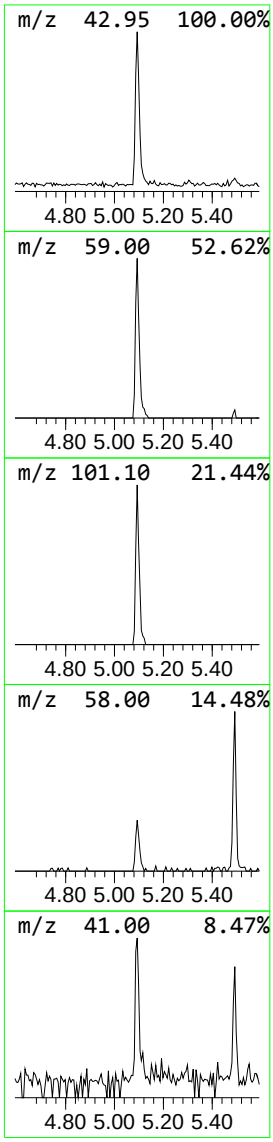
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.01 ng	54355	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	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133813.D
Acq On : 16 Jun 2023 18:36
Operator : CG\JU
Sample : 03223-13 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-11

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

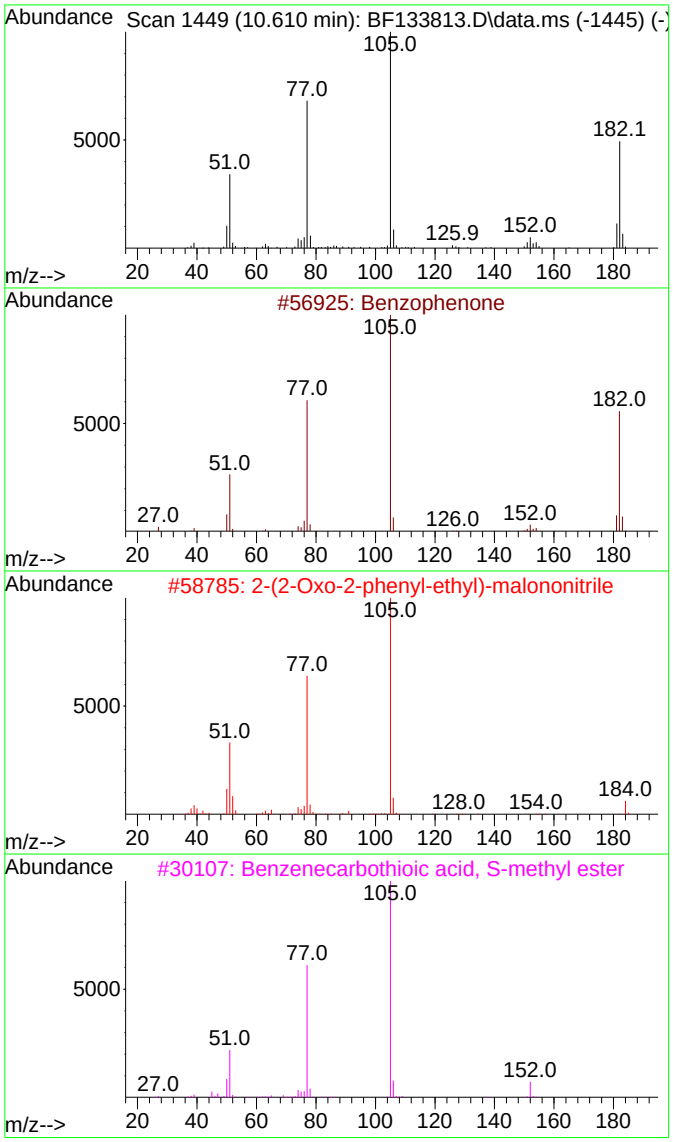
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

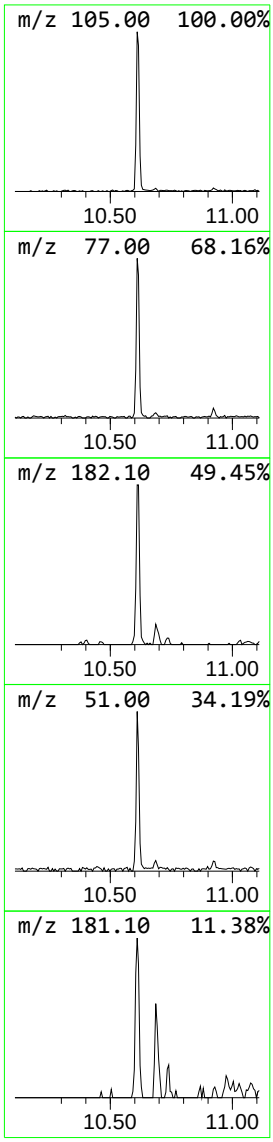
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	3.62 ng	125195	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	53
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
5	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133813.D
Acq On : 16 Jun 2023 18:36
Operator : CG\JU
Sample : 03223-13 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-11

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

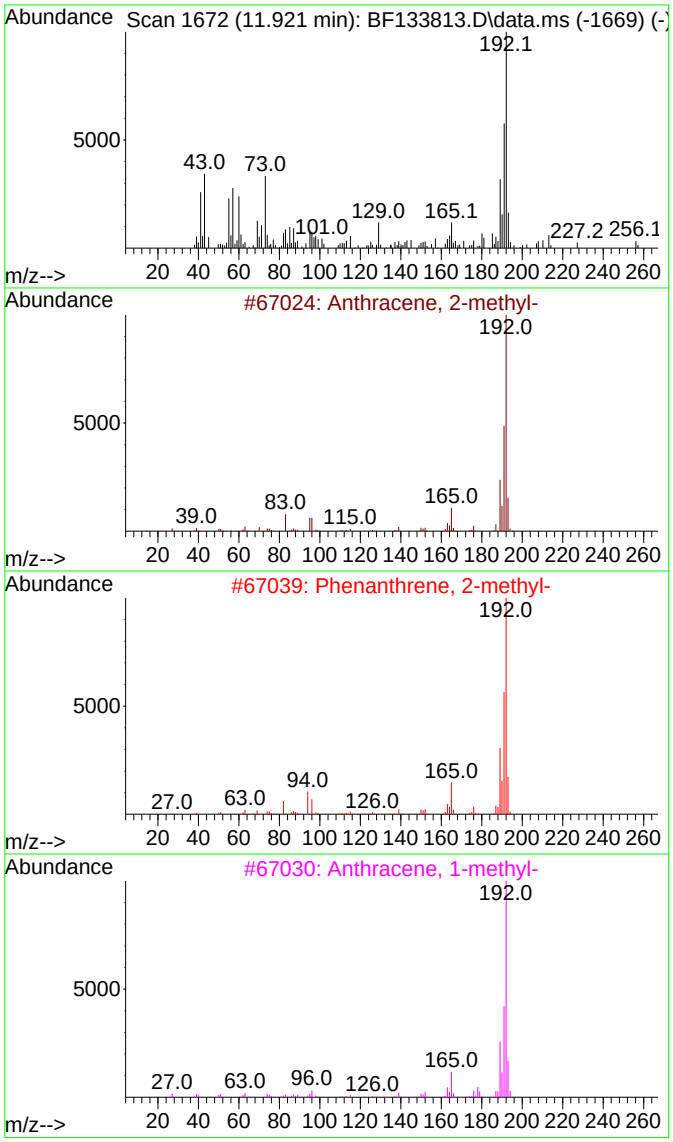
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

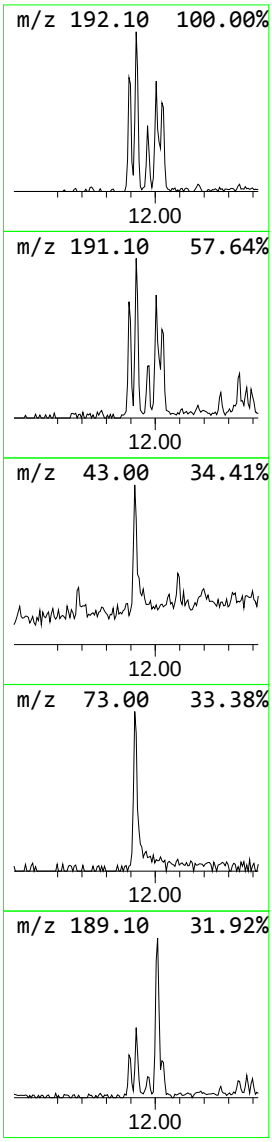
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.44 ng	119305	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133813.D
Acq On : 16 Jun 2023 18:36
Operator : CG\JU
Sample : 03223-13 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-11

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

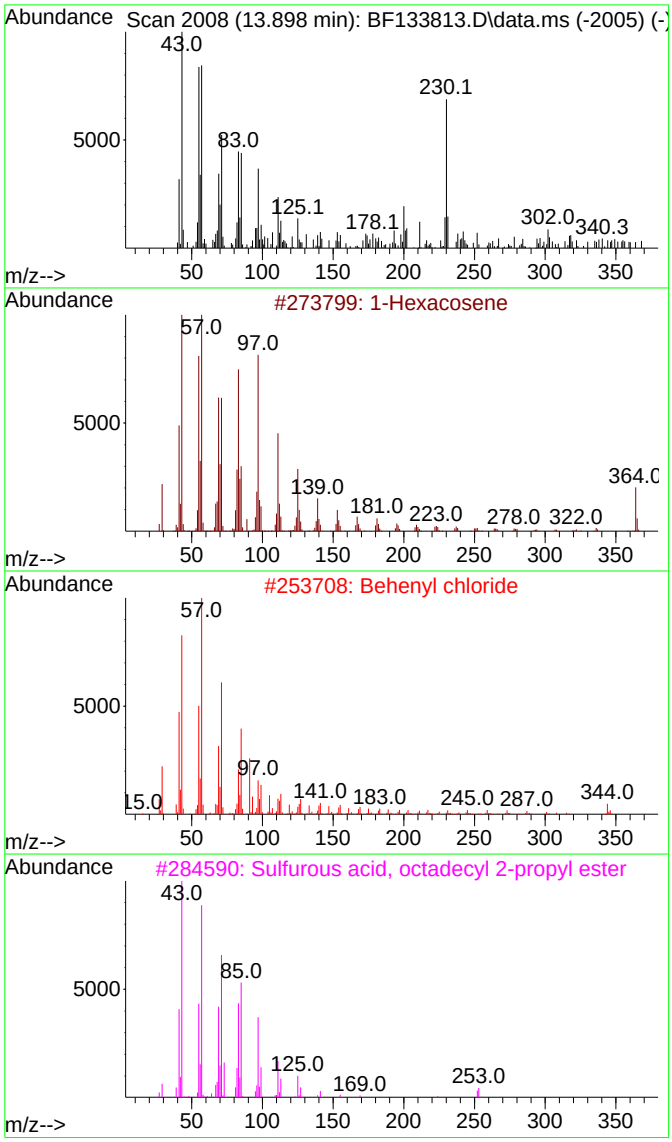
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

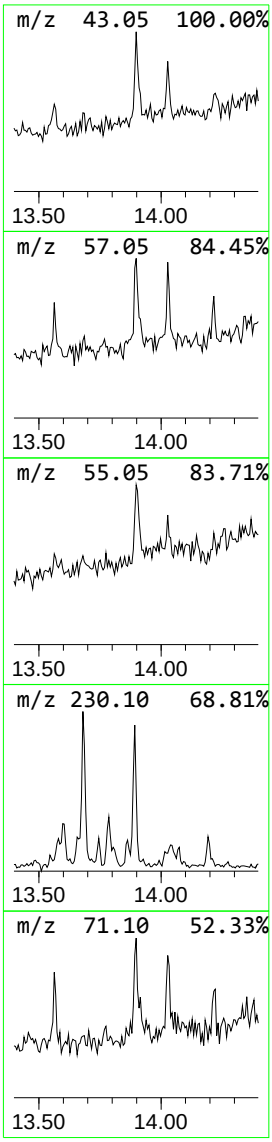
****

Peak Number 5 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.25 ng	84194	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	89
2	Behenyl chloride	344	C22H45Cl	042217-03-8	55
3	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	53
4	Tetracosane	338	C24H50	000646-31-1	51
5	Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133813.D
Acq On : 16 Jun 2023 18:36
Operator : CG\JU
Sample : 03223-13 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-11

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

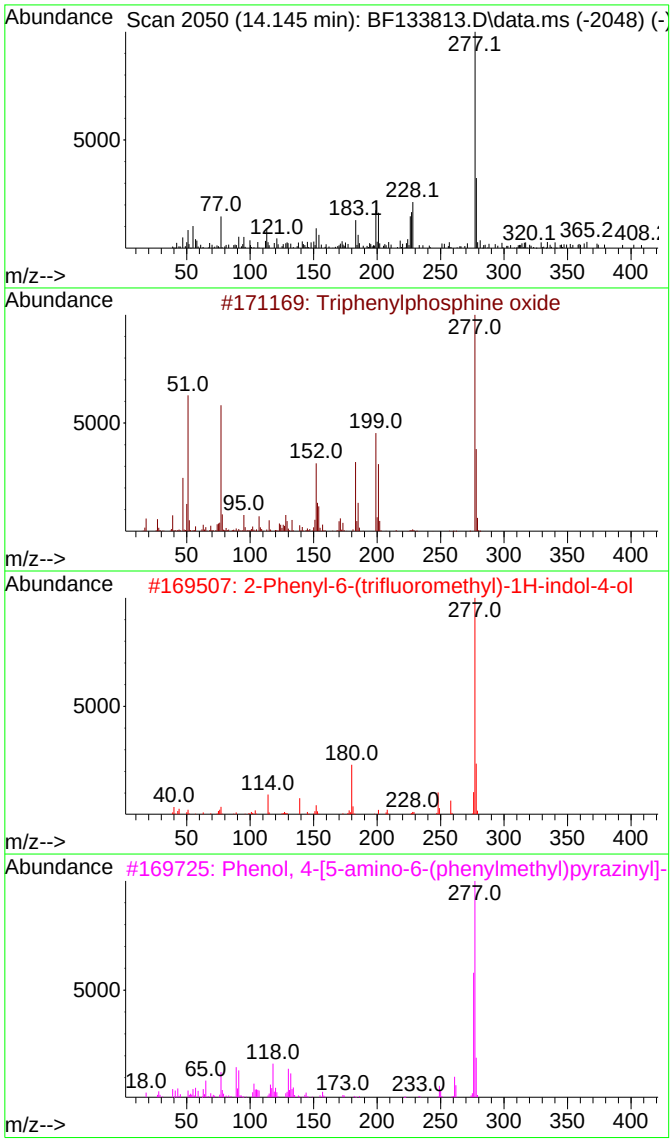
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

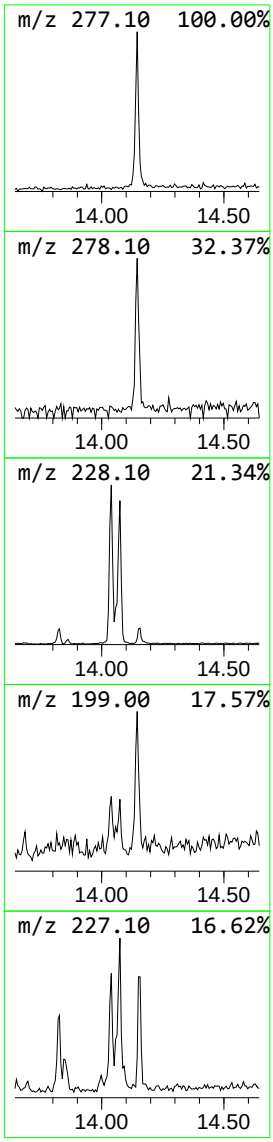
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.145	2.00 ng	74824	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	83
2	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	50
3	Phenol, 4-[5-amino-6-(phenylmeth...	277	C17H15N3O	037156-84-6	43
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	43
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133813.D
Acq On : 16 Jun 2023 18:36
Operator : CG\JU
Sample : 03223-13 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-11

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...	2.140	3.9	ng	104630	1	6.863	540392	20.0
2-Pentanone, 4-...	5.093	2.0	ng	54355	1	6.863	540392	20.0
Benzophenone	10.610	3.6	ng	125195	3	9.898	692196	20.0
Anthracene, 2-m...	11.922	3.4	ng	119305	4	11.392	692742	20.0
1-Hexacosene	13.898	2.3	ng	84194	5	14.051	747619	20.0
Triphenylphosph...	14.145	2.0	ng	74824	5	14.051	747619	20.0