LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100324\
Data File : BF139641.D
Acq On : 03 Oct 2024 19:50
Operator : RC/JU
Sample : P4236-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

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-BF100124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139641.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	5	14	21	rVB	1678386	2700421	100.00%	13.937%
2	2.505	61	70	78	rVB	13732	32762	1.21%	0.169%
3	5.081	499	508	517	rVB	107292	171492	6.35%	0.885%
4	5.487	571	577	582	rBV	1452042	1883599	69.75%	9.721%
5	6.492	742	748	764	rVB	1450920	1951101	72.25%	10.070%
6	6.863	806	811	816	rBV	430947	518776	19.21%	2.677%
7	7.428	900	907	912	rBV	941289	1271630	47.09%	6.563%
8	8.145	1023	1029	1041	rBV	538420	673238	24.93%	3.475%
9	9.222	1206	1212	1217	rBV	1655615	2118030	78.43%	10.931%
10	9.898	1322	1327	1332	rBV	609185	750221	27.78%	3.872%
11	10.610	1443	1448	1456	rVB	78947	100900	3.74%	0.521%
12	10.686	1456	1461	1472	rBV	1016314	1305053	48.33%	6.735%
13	11.386	1575	1580	1588	rBV2	617924	971909	35.99%	5.016%
14	11.457	1588	1592	1596	rVB	36762	47623	1.76%	0.246%
15	11.910	1660	1669	1675	rBV2	161061	270672	10.02%	1.397%
16	11.998	1680	1684	1693	rVB	53705	106059	3.93%	0.547%
17	12.433	1754	1758	1762	rBV	24037	37236	1.38%	0.192%
18	12.469	1762	1764	1770	rVV3	17396	30053	1.11%	0.155%
19	12.598	1781	1786	1791	rBV	230427	283354	10.49%	1.462%
20	12.827	1815	1825	1830	rBV	205148	305336	11.31%	1.576%
21	12.969	1840	1849	1856	rVB	1383313	1802535	66.75%	9.303%
22	13.045	1856	1862	1869	rBV3	20096	39019	1.44%	0.201%
23	13.151	1873	1880	1884	rVB2	28485	53599	1.98%	0.277%
24	13.574	1941	1952	1956	rBV10	7956	29144	1.08%	0.150%
25	13.663	1960	1967	1972	rVV2	16253	28238	1.05%	0.146%
26	13.774	1980	1986	1988	rBV2	16670	28320	1.05%	0.146%
27	13.874	1999	2003	2020	rVB3	49631	116345	4.31%	0.600%
28	14.021	2020	2028	2039	rVB2	442082	757537	28.05%	3.910%
29	15.063	2200	2205	2214	rBV	77888	178488	6.61%	0.921%
30	15.368	2252	2257	2262	rVB	43091	63580	2.35%	0.328%
31	15.427	2262	2267	2272	rVB	61227	89369	3.31%	0.461%
32	15.492	2272	2278	2292	rVB	329292	538268	19.93%	2.778%
33	16.957	2520	2527	2537	rVB2	29824	68745	2.55%	0.355%
34	17.398	2595	2602	2612	rVB2	23622	53506	1.98%	0.276%

Sum of corrected areas: 19376158

Instrument :
BNA_F
ClientSampleId :
TP1

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100324\
Data File : BF139641.D
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Operator : RC/JU
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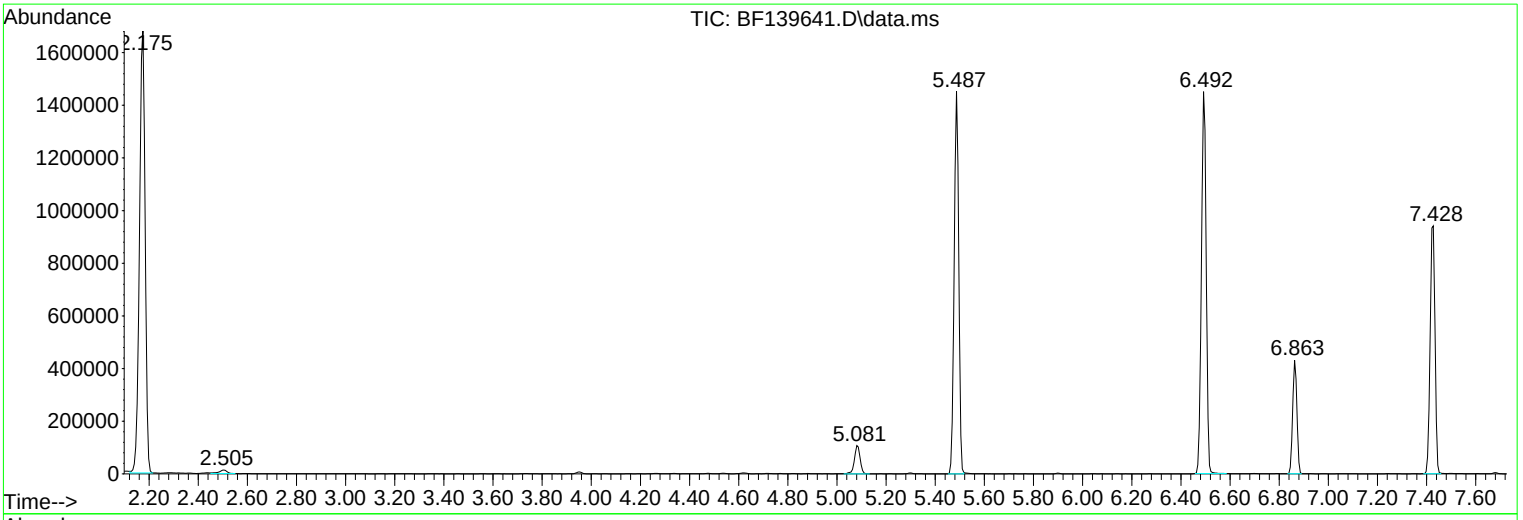
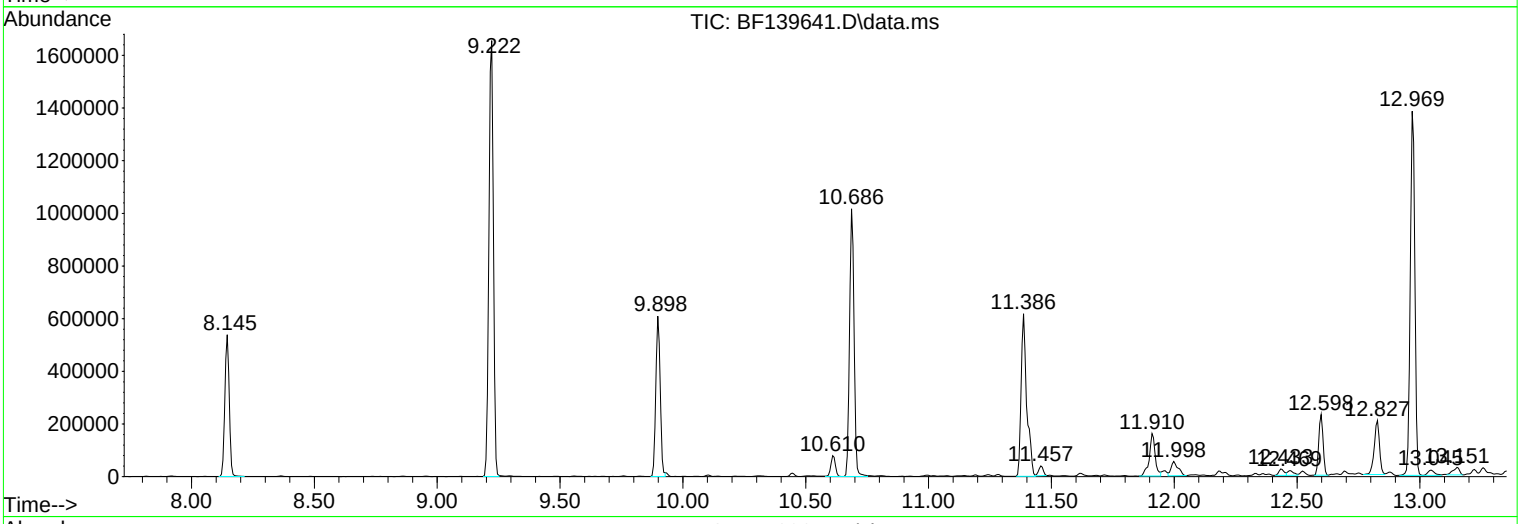
Misc :
ALS Vial : 23 Sample Multiplier: 1

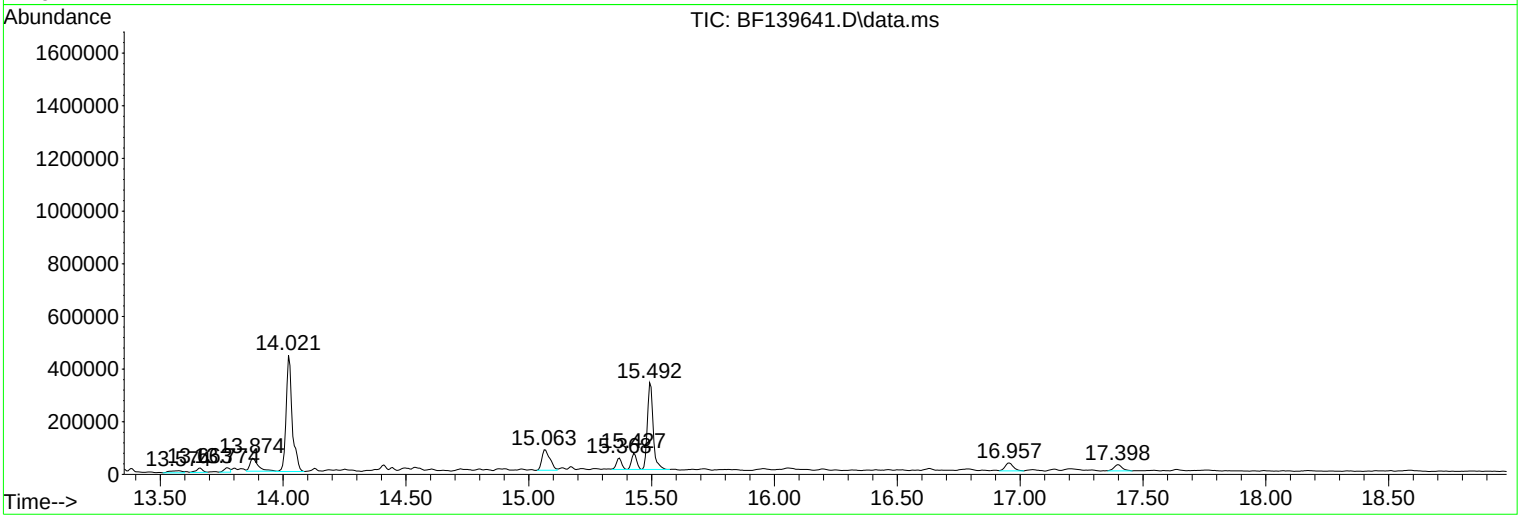
Instrument :
BNA_F
ClientSampleId :
TP1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

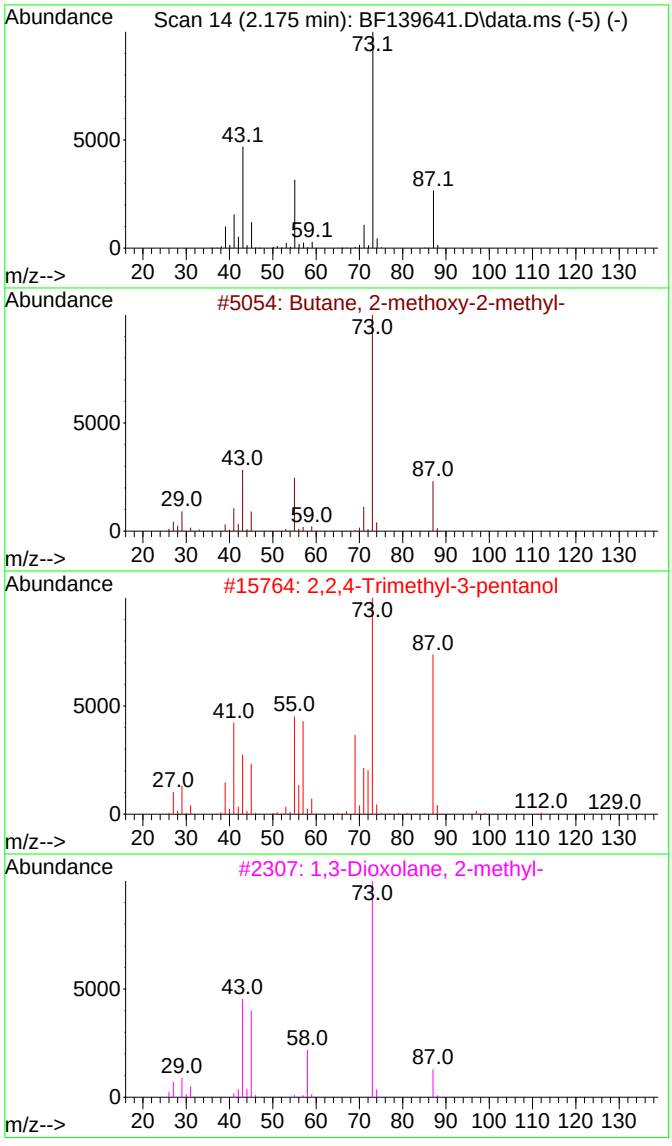
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

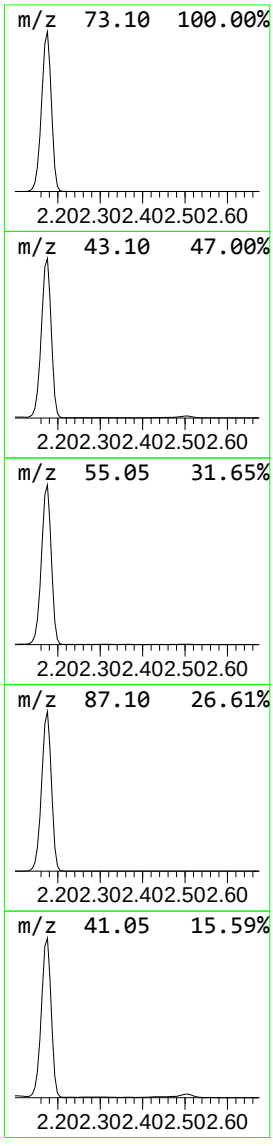
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	104.11 ng	2700420	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	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Data File : BF139641.D
Acq On : 03 Oct 2024 19:50
Operator : RC/JU
Sample : P4236-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

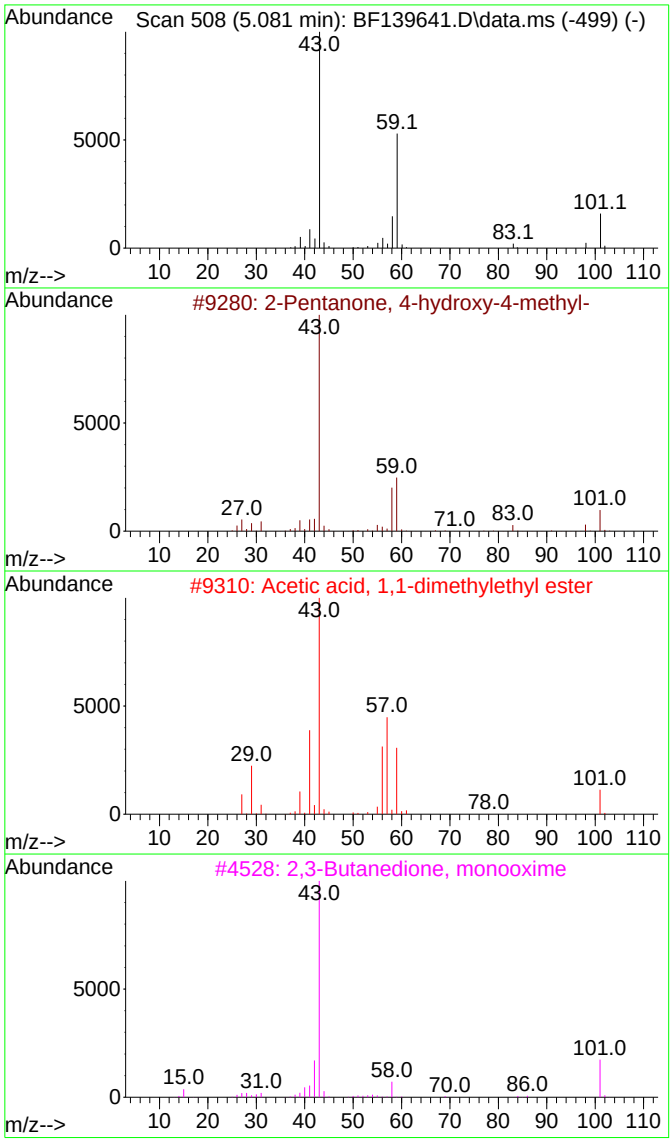
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

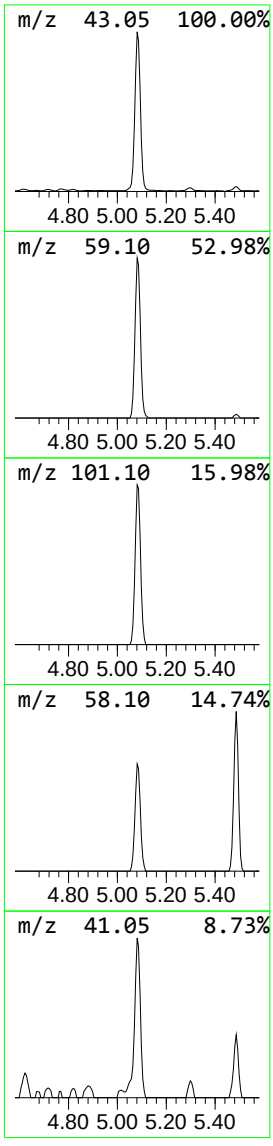
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	6.61 ng	171492	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25





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Sample : P4236-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

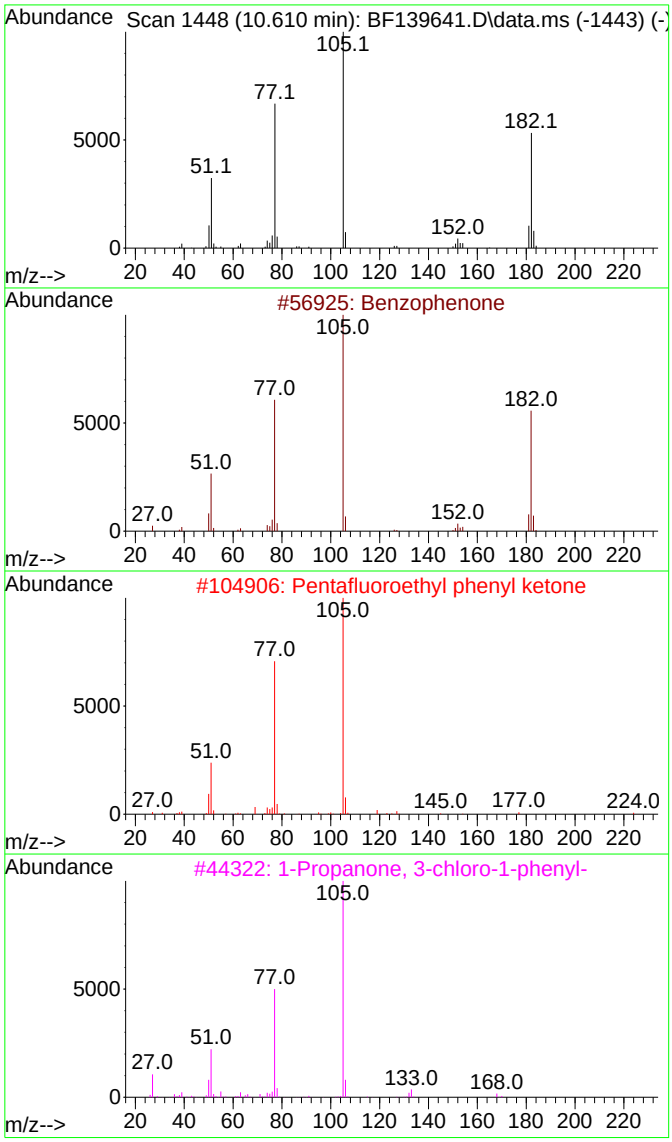
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

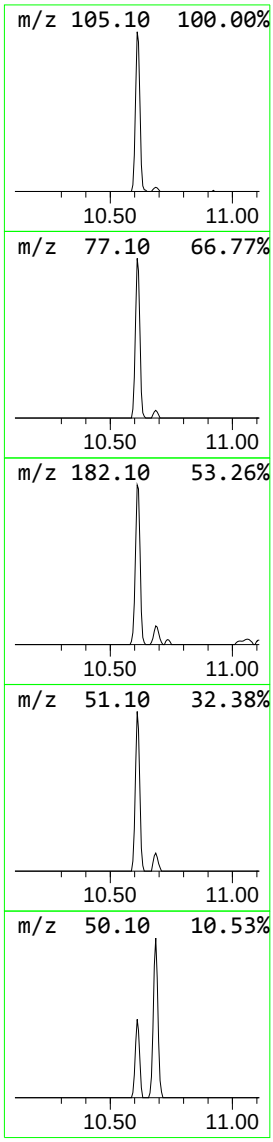
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	2.69 ng	100900	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
4	Vinyl benzoate	148	C9H8O2	000769-78-8	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





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Sample : P4236-09
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Instrument :
BNA_F
ClientSampleId :
TP1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

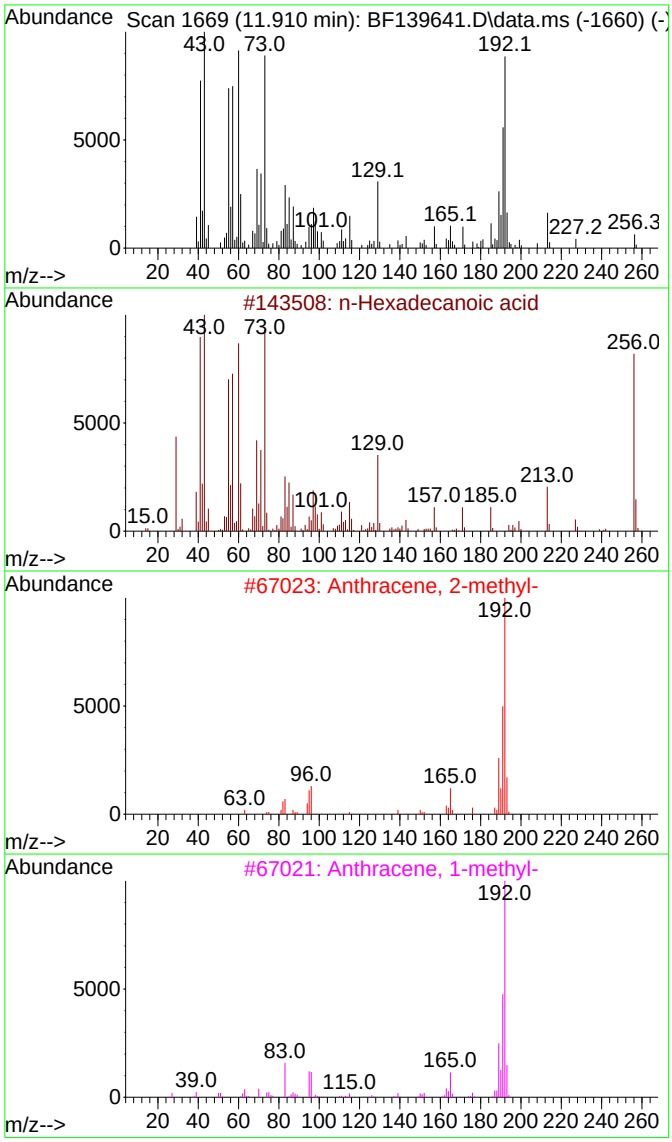
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

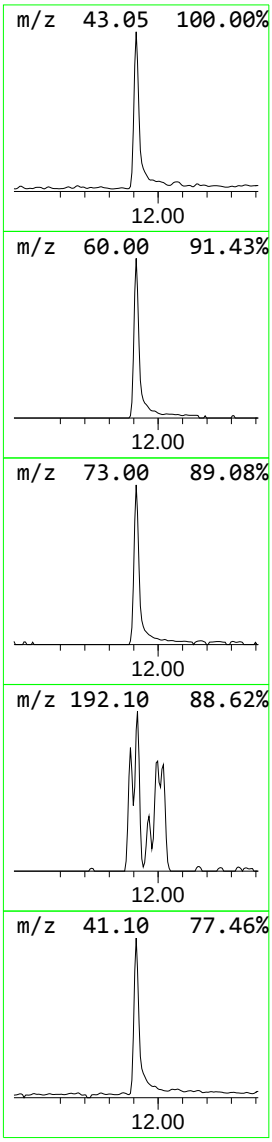
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	5.57 ng	270672	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	92
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	78
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100324\
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Sample : P4236-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1

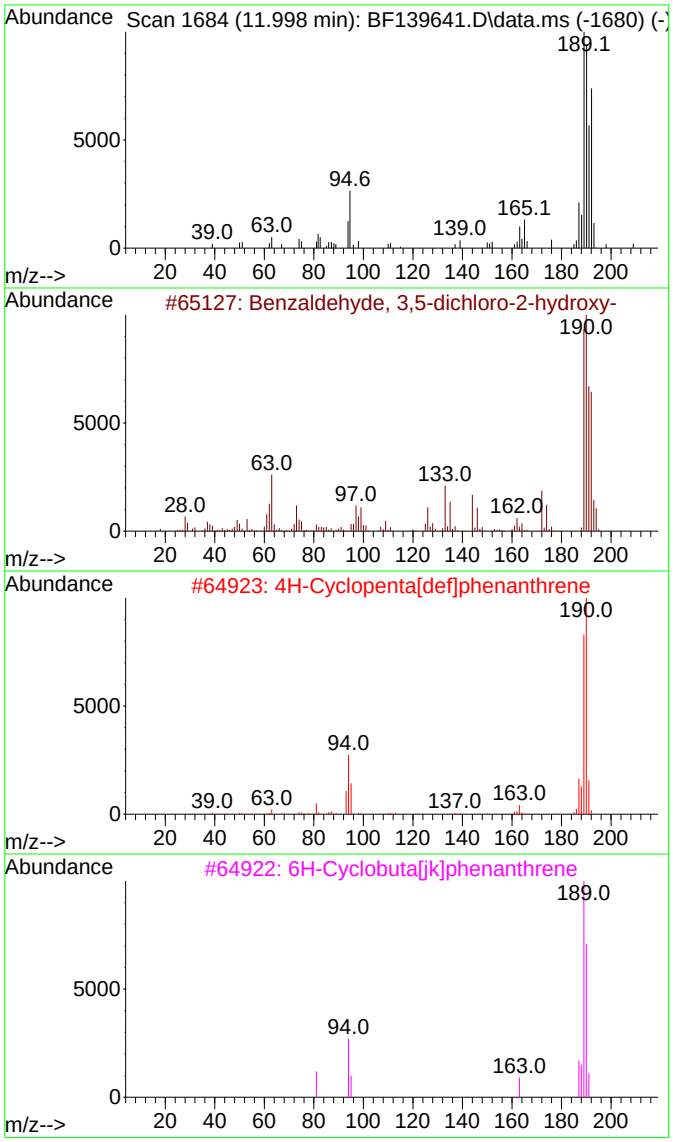
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

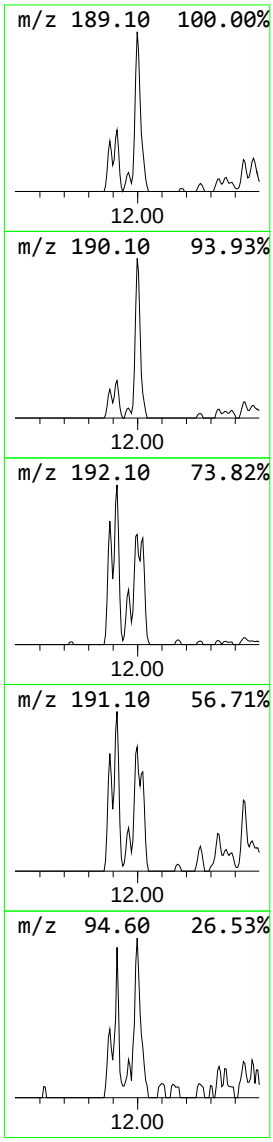
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzaldehyde, 3,5-dichloro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	2.18 ng	106059	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
4	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	38
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38





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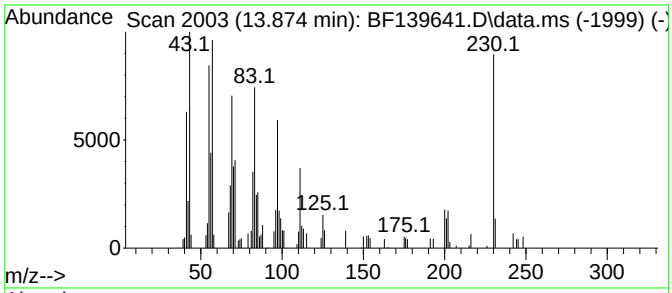
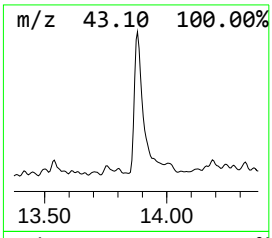
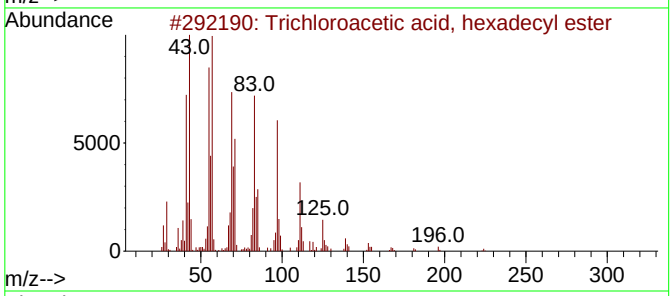
****
Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 4

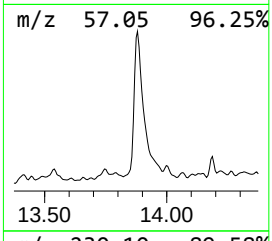
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.07 ng	116345	Chrysene-d12	14.021

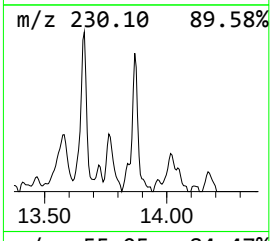
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93

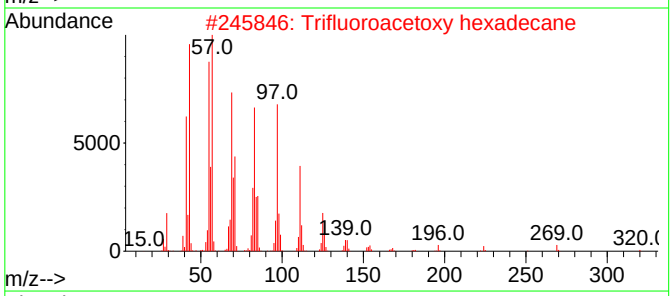


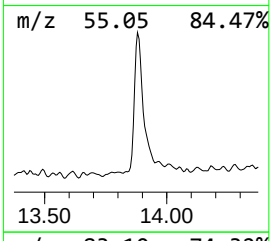


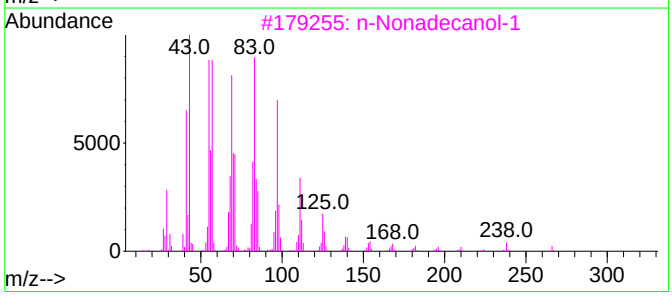


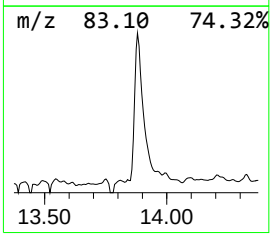












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

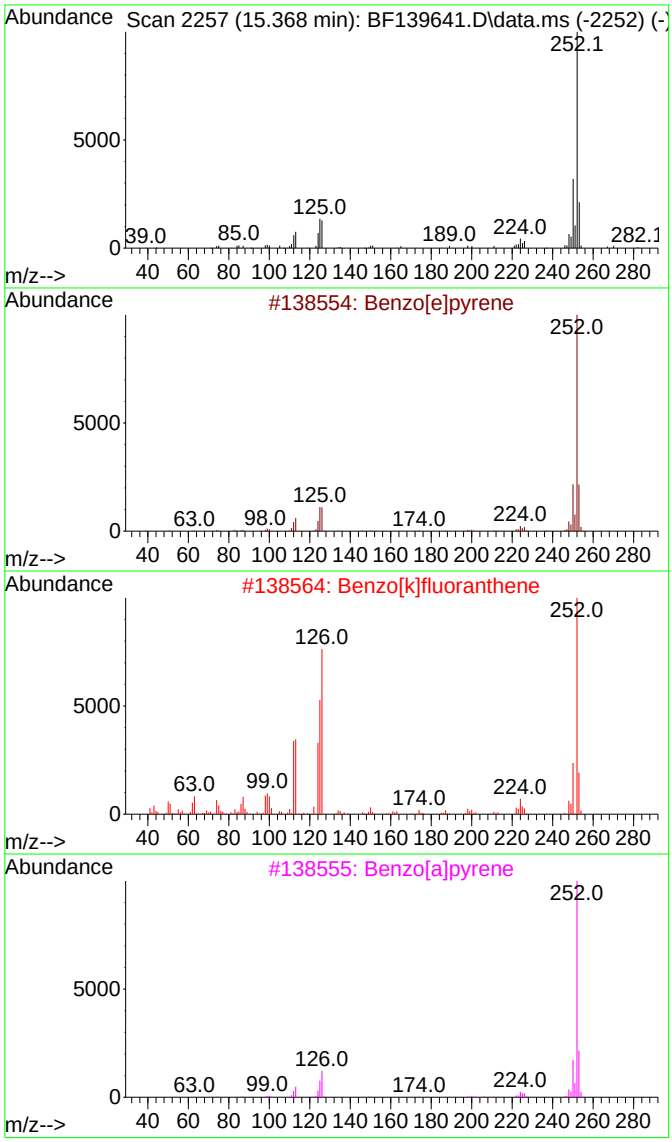
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

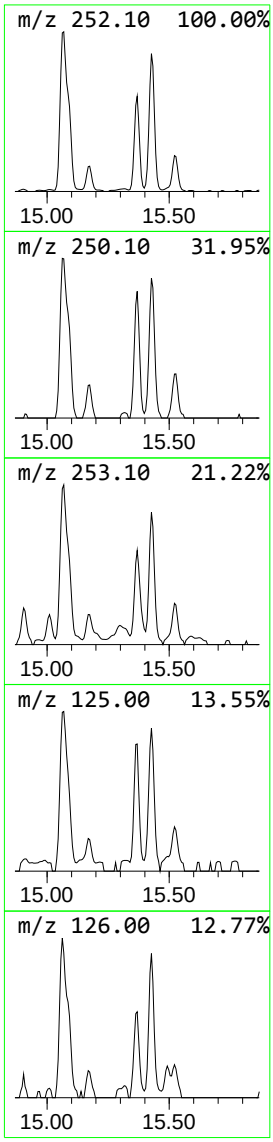
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.368	2.36 ng	63580	Perylene-d12	15.492

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	Benzo[a]pyrene	252	C20H12	000050-32-8	91
4	Perylene	252	C20H12	000198-55-0	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Tentatively Identified Compound (LSC) summary

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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...	2.175	104.1	ng	2700420	1	6.863	518776	20.0
2-Pentanone, 4-...	5.081	6.6	ng	171492	1	6.863	518776	20.0
Benzophenone	10.610	2.7	ng	100900	3	9.898	750221	20.0
n-Hexadecanoic ...	11.910	5.6	ng	270672	4	11.386	971909	20.0
Benzaldehyde, 3...	11.998	2.2	ng	106059	4	11.386	971909	20.0
Trichloroacetic...	13.874	3.1	ng	116345	5	14.021	757537	20.0
Benzo[e]pyrene	15.368	2.4	ng	63580	6	15.492	538268	20.0