LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100424\
Data File : BF139674.D
Acq On : 04 Oct 2024 23:07
Operator : RC/JU
Sample : P4276-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

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: BF139674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	23	rVB	1447505	2212587	100.00%	14.879%
2	5.075	497	507	525	rVB	74600	114346	5.17%	0.769%
3	5.487	571	577	594	rVB	1064918	1443397	65.24%	9.706%
4	6.493	742	748	772	rBV	1094595	1490185	67.35%	10.021%
5	6.863	806	811	816	rBV	417578	507243	22.93%	3.411%
6	7.428	901	907	912	rBV	718767	949054	42.89%	6.382%
7	7.681	945	950	960	rBV	35539	47977	2.17%	0.323%
8	8.145	1024	1029	1044	rVB	492750	612498	27.68%	4.119%
9	9.222	1206	1212	1217	rBV	1192471	1519885	68.69%	10.221%
10	9.898	1322	1327	1331	rBV	463594	569003	25.72%	3.826%
11	10.233	1378	1384	1389	rBV4	20180	46153	2.09%	0.310%
12	10.298	1392	1395	1398	rBV2	22876	33091	1.50%	0.223%
13	10.610	1443	1448	1455	rBV	324050	419663	18.97%	2.822%
14	10.686	1456	1461	1466	rBV	551619	708625	32.03%	4.765%
15	10.810	1478	1482	1488	rBV	45189	87802	3.97%	0.590%
16	10.922	1498	1501	1509	rBV2	63911	132008	5.97%	0.888%
17	10.992	1510	1513	1516	rBV2	44765	70357	3.18%	0.473%
18	11.128	1533	1536	1538	rBV2	39430	55880	2.53%	0.376%
19	11.386	1576	1580	1584	rBV	423743	590563	26.69%	3.971%
20	11.916	1667	1670	1676	rBV2	131728	173864	7.86%	1.169%
21	12.974	1846	1850	1859	rBV2	1097990	1627395	73.55%	10.943%
22	14.663	2133	2137	2141	rBV	1069968	1459323	65.96%	9.813%

Sum of corrected areas: 14870899

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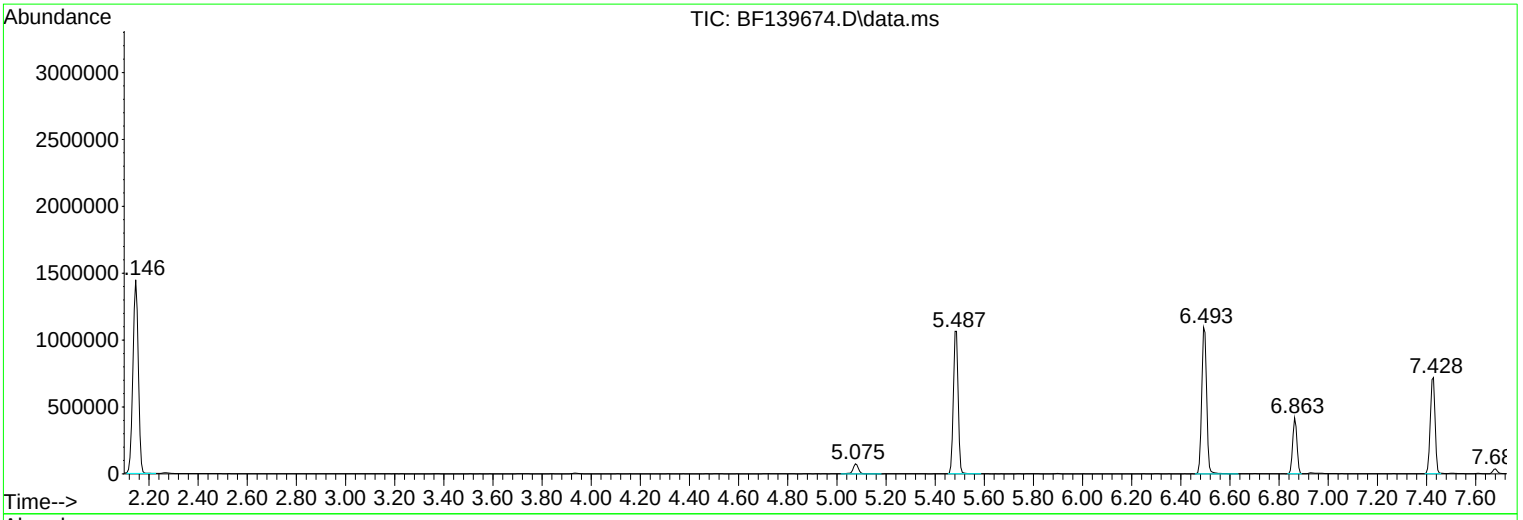
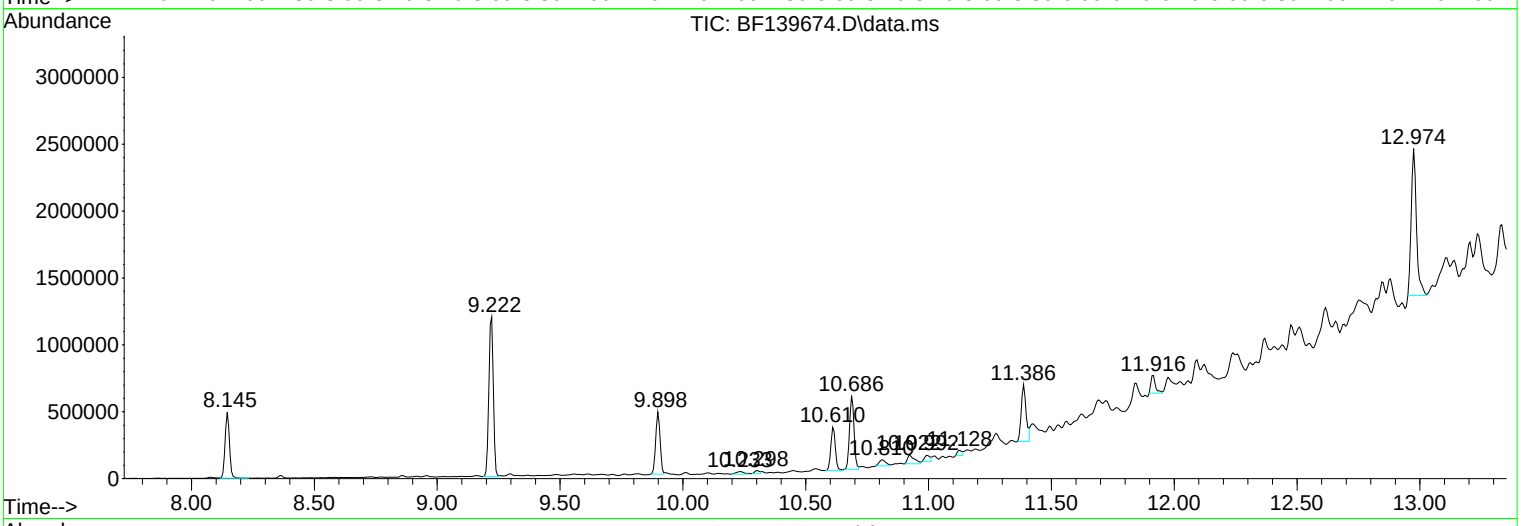
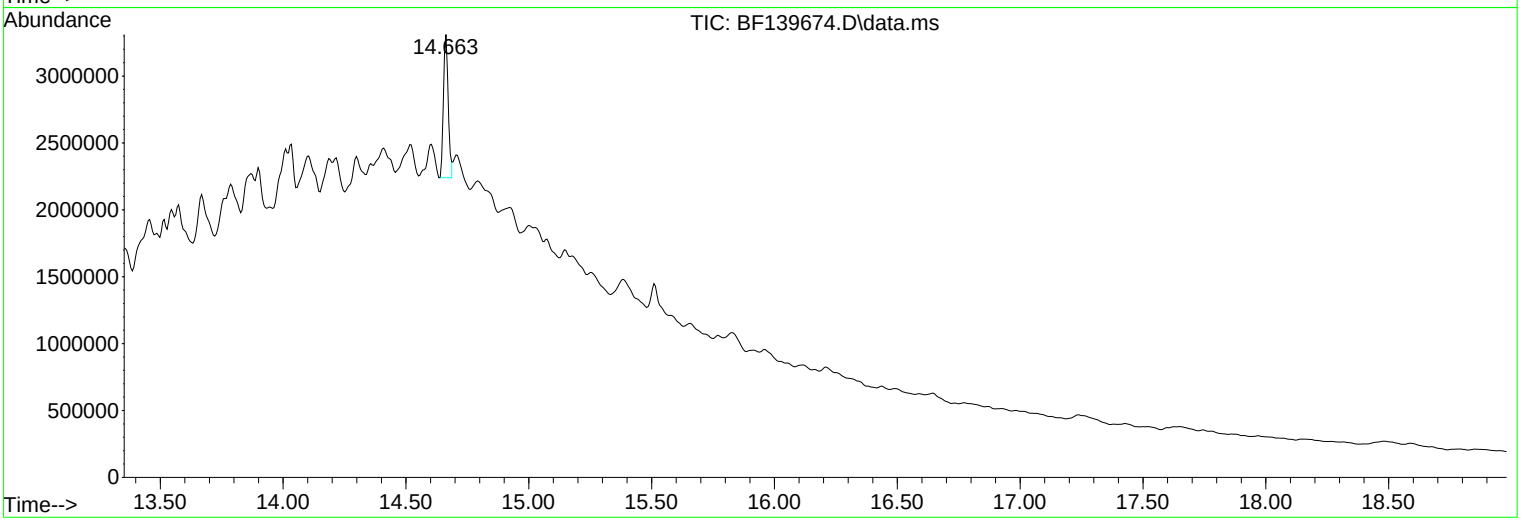
Instrument :
BNA_F
ClientSampleId :
VNJ-208

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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ClientSampleId :
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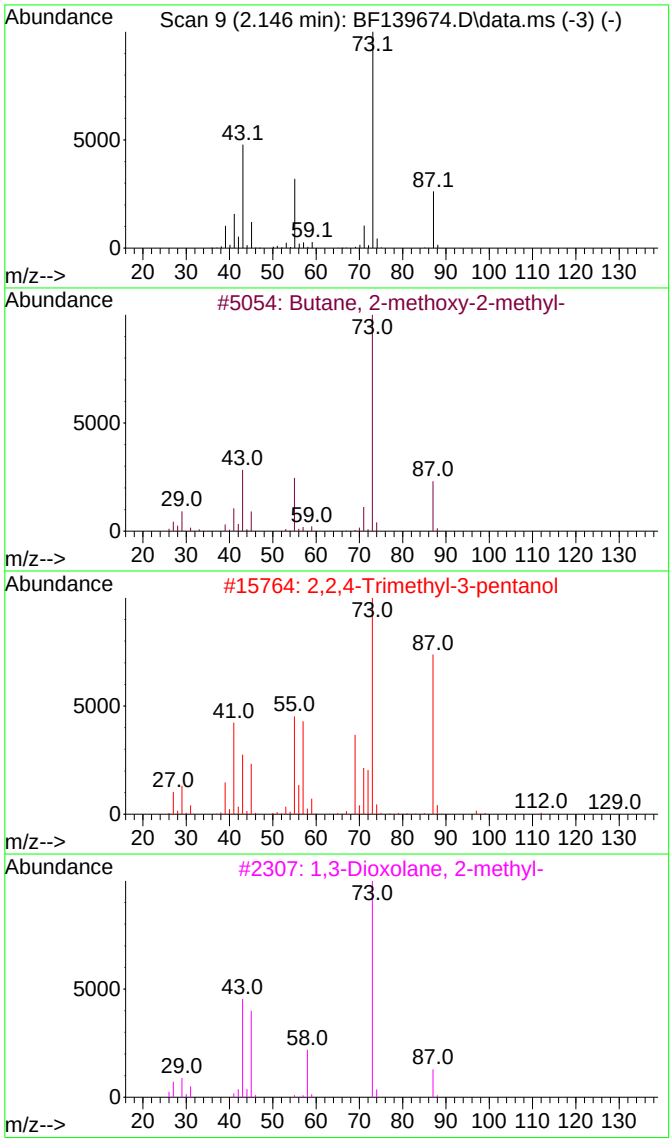
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

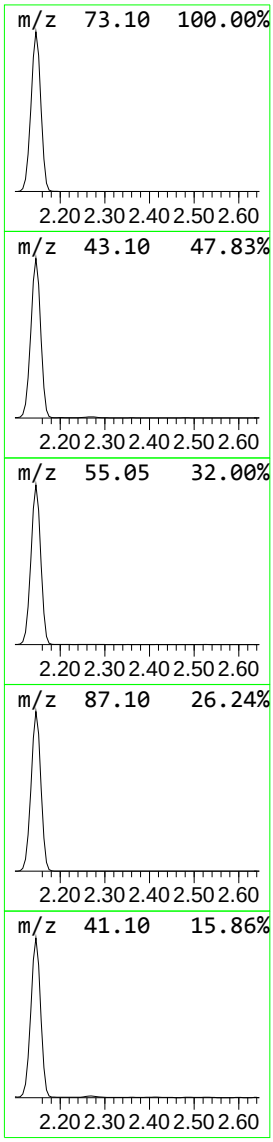
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	87.24 ng	2212590	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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Operator : RC/JU
Sample : P4276-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

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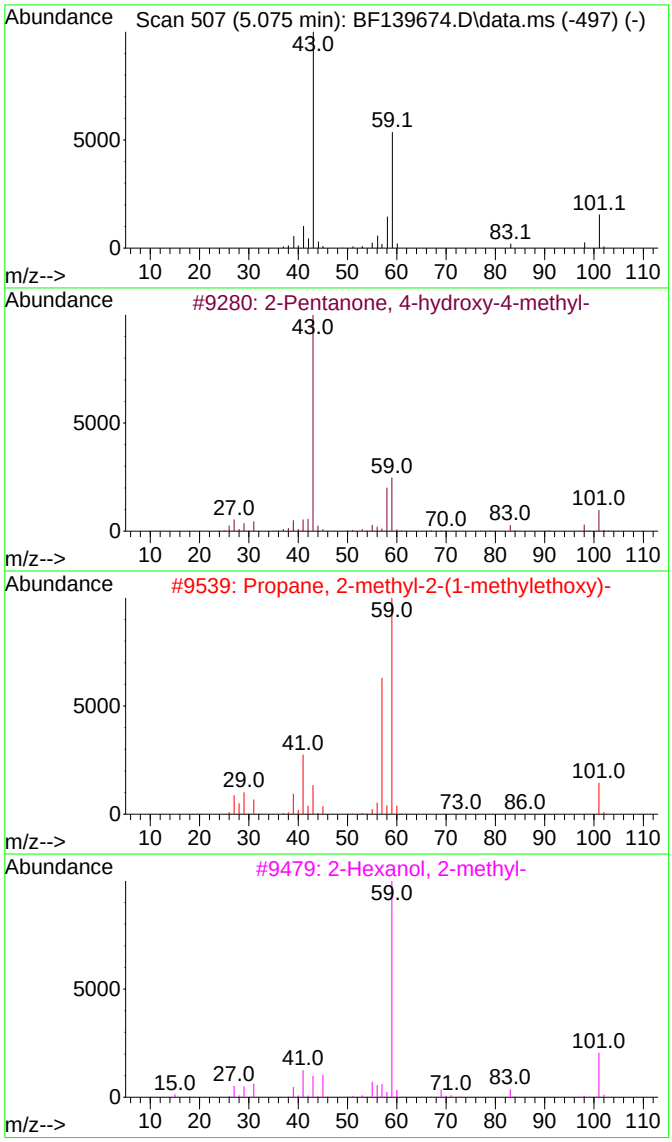
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

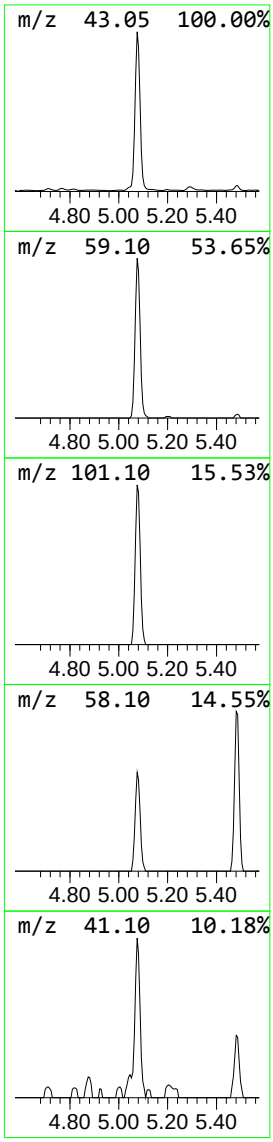
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	4.51 ng	114346	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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





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Sample : P4276-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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
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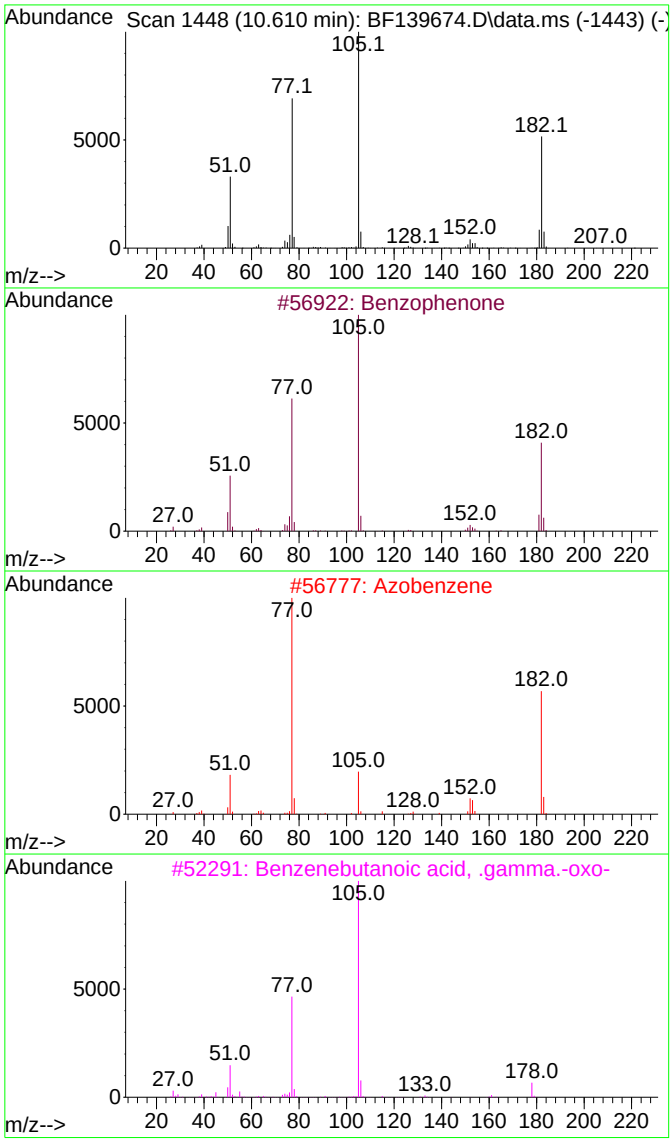
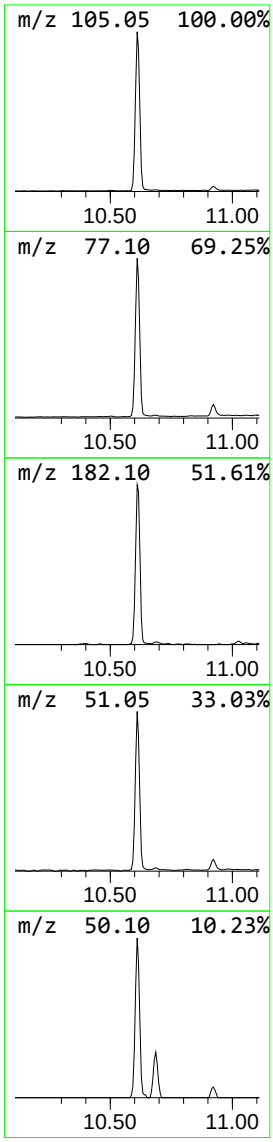
****

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	14.75 ng	419663	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	58
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
4	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50
5	N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50





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Sample : P4276-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

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

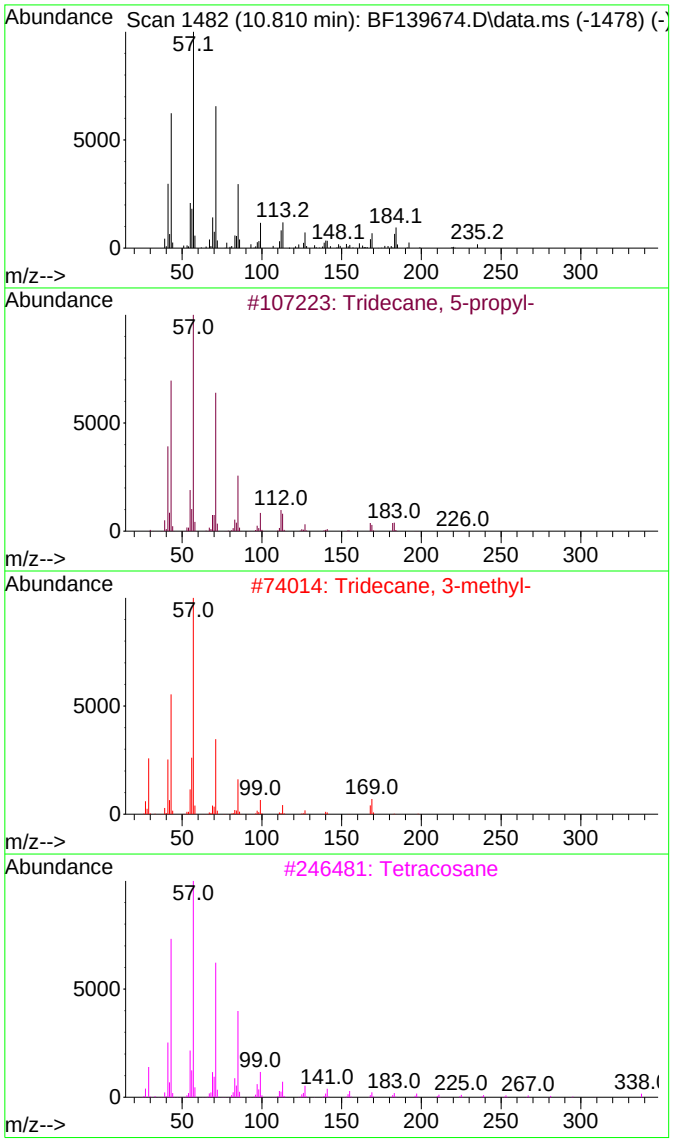
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

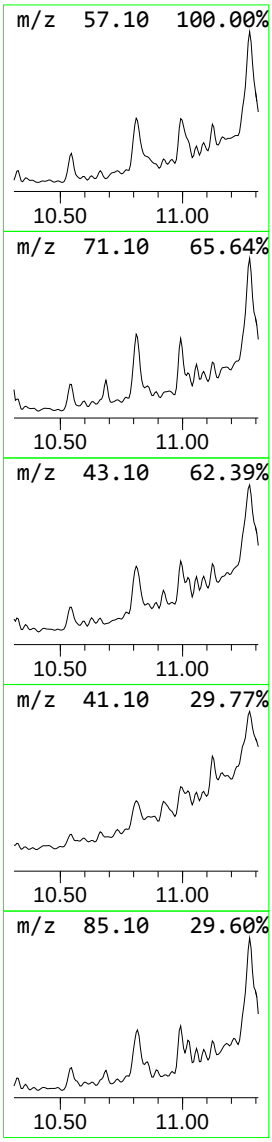
****

Peak Number 4 Tridecane, 5-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.810	2.97 ng	87802	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	80
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	72
3	Tetracosane	338	C24H50	000646-31-1	64
4	Heptacosane	380	C27H56	000593-49-7	64
5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	64





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Sample : P4276-01
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ALS Vial : 24 Sample Multiplier: 1

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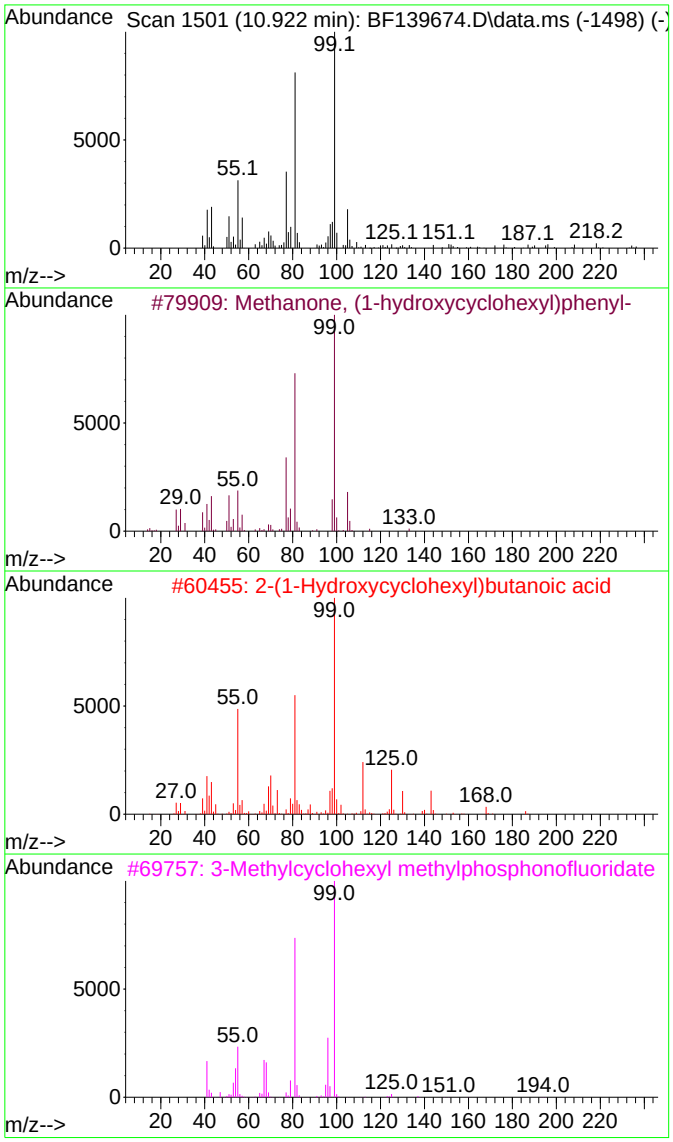
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

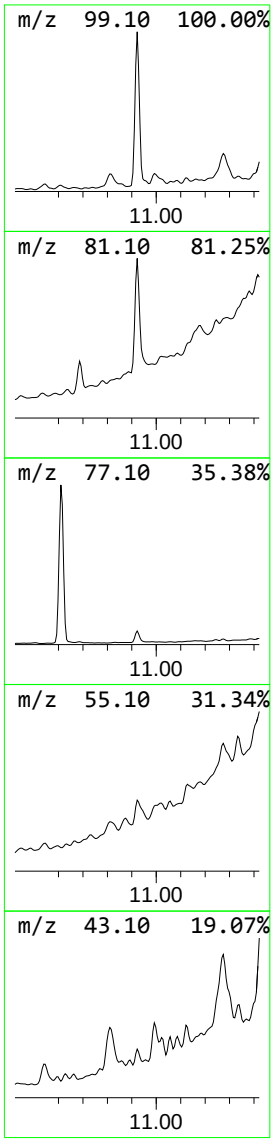
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Methanone, (1-hydroxycycloh... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.922	4.47 ng	132008	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	87
2	2-(1-Hydroxycyclohexyl)butanoic ...	186	C10H18O3	000512-16-3	64
3	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	59
4	2,2'-Bioxepane	198	C12H22O2	074793-02-5	59
5	2-Methylcyclosarin	194	C8H16FO2P	085473-32-1	50





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TIC Library : C:\Database\NIST20.L
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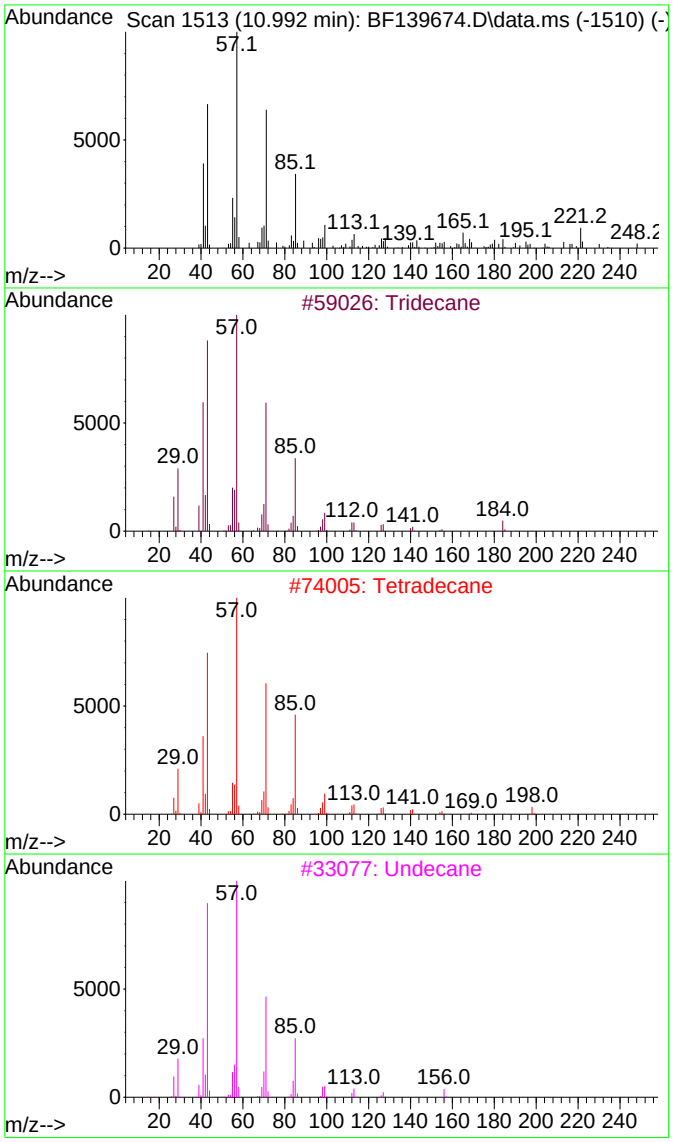
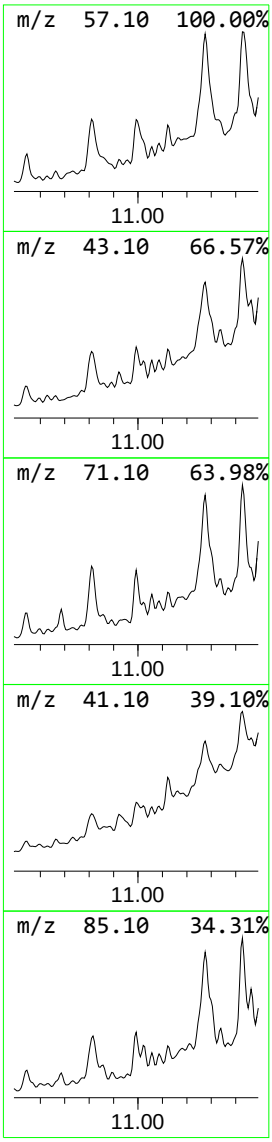
****

Peak Number 6 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.992	2.38 ng	70357	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Tetradecane	198	C14H30	000629-59-4	68
3	Undecane	156	C11H24	001120-21-4	68
4	Nonadecane	268	C19H40	000629-92-5	64
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
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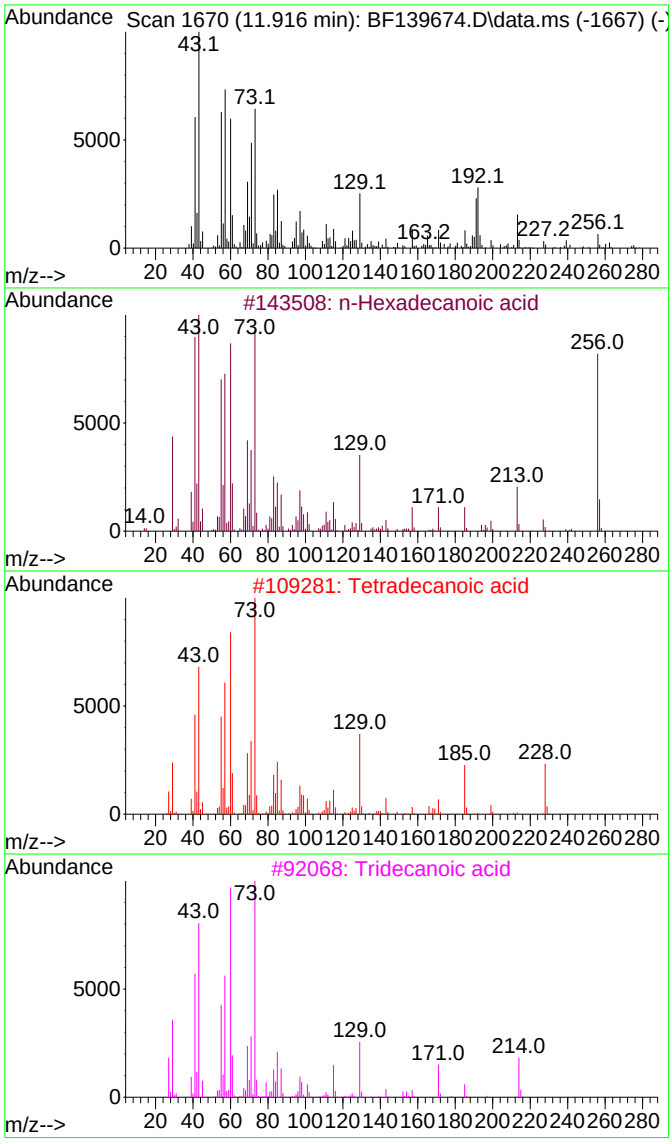
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

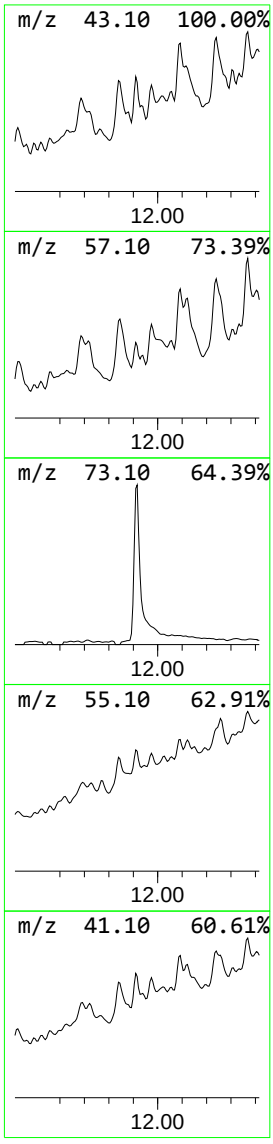
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	5.89 ng	173864	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
3	Tridecanoic acid	214	C13H26O2	000638-53-9	46
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	42





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TIC Library : C:\Database\NIST20.L
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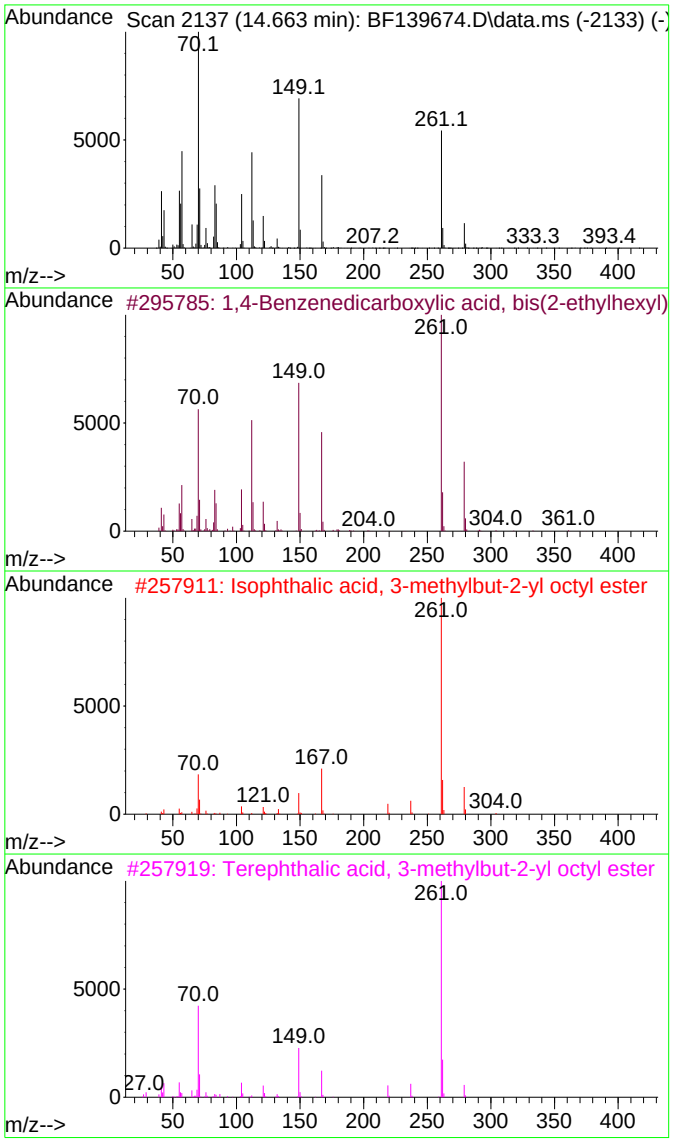
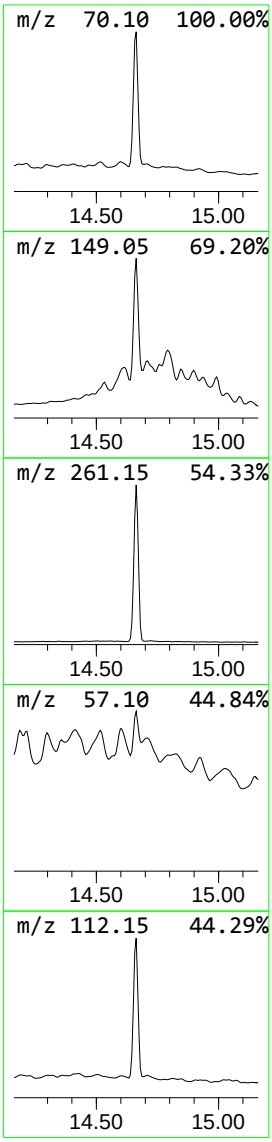
****
Peak Number 8 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.663	20.00 ng	1459320	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
2	Isophthalic acid, 3-methylbut-2-...	348	C21H32O4	1000344-72-4	50
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	49
4	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	49
5	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.146	87.2	ng	2212590	1	6.863	507243	20.0
2-Pentanone, 4-...	5.075	4.5	ng	114346	1	6.863	507243	20.0
Benzophenone	10.610	14.8	ng	419663	3	9.898	569003	20.0
Tridecane, 5-pr...	10.810	3.0	ng	87802	4	11.386	590563	20.0
Methanone, (1-h...	10.922	4.5	ng	132008	4	11.386	590563	20.0
Tridecane	10.992	2.4	ng	70357	4	11.386	590563	20.0
n-Hexadecanoic ...	11.916	5.9	ng	173864	4	11.386	590563	20.0
1,4-Benzenedica...	14.663	20.0	ng	1459320	5	14.033	1459320	20.0