LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130868.D
Acq On : 29 Oct 2022 20:50
Operator : CG\JU
Sample : N5307-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-102622

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130868.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	23	30	36	rVB	987440	1266306	73.48%	9.249%
2	2.375	45	49	57	rVB	46349	63595	3.69%	0.464%
3	5.175	520	525	534	rVB	521335	600222	34.83%	4.384%
4	5.563	586	591	594	rBV	1834313	1723249	100.00%	12.586%
5	6.563	756	761	764	rBV	1729689	1630398	94.61%	11.908%
6	6.587	764	765	773	rVB	32405	31523	1.83%	0.230%
7	6.945	823	826	830	rVB	529831	421448	24.46%	3.078%
8	7.510	917	922	925	rBV	1119596	940027	54.55%	6.866%
9	8.234	1041	1045	1048	rBV	568518	456278	26.48%	3.332%
10	9.310	1223	1228	1231	rBV	1855015	1534134	89.03%	11.205%
11	9.851	1317	1320	1323	rVB	47749	41143	2.39%	0.300%
12	9.992	1340	1344	1347	rVB	587053	457619	26.56%	3.342%
13	10.781	1474	1478	1482	rBV	1218075	994391	57.70%	7.263%
14	10.904	1494	1499	1502	rBV6	22321	32991	1.91%	0.241%
15	11.486	1594	1598	1600	rBV	599166	494316	28.69%	3.610%
16	11.510	1600	1602	1605	rVB	109348	86907	5.04%	0.635%
17	11.557	1606	1610	1613	rVV	44331	49293	2.86%	0.360%
18	11.869	1661	1663	1666	rVB2	30295	20791	1.21%	0.152%
19	11.998	1681	1685	1686	rBV2	56882	65754	3.82%	0.480%
20	12.098	1699	1702	1705	rBV2	51895	59034	3.43%	0.431%
21	12.704	1802	1805	1808	rBV	295791	273398	15.87%	1.997%
22	12.933	1841	1844	1849	rVB	339665	285444	16.56%	2.085%
23	13.075	1864	1868	1871	rBV	1741315	1421347	82.48%	10.381%
24	13.257	1897	1899	1903	rVB2	73306	63782	3.70%	0.466%
25	14.133	2044	2048	2051	rBV2	428056	502258	29.15%	3.668%
26	14.227	2062	2064	2068	rVB2	181576	176122	10.22%	1.286%

Sum of corrected areas: 13691770

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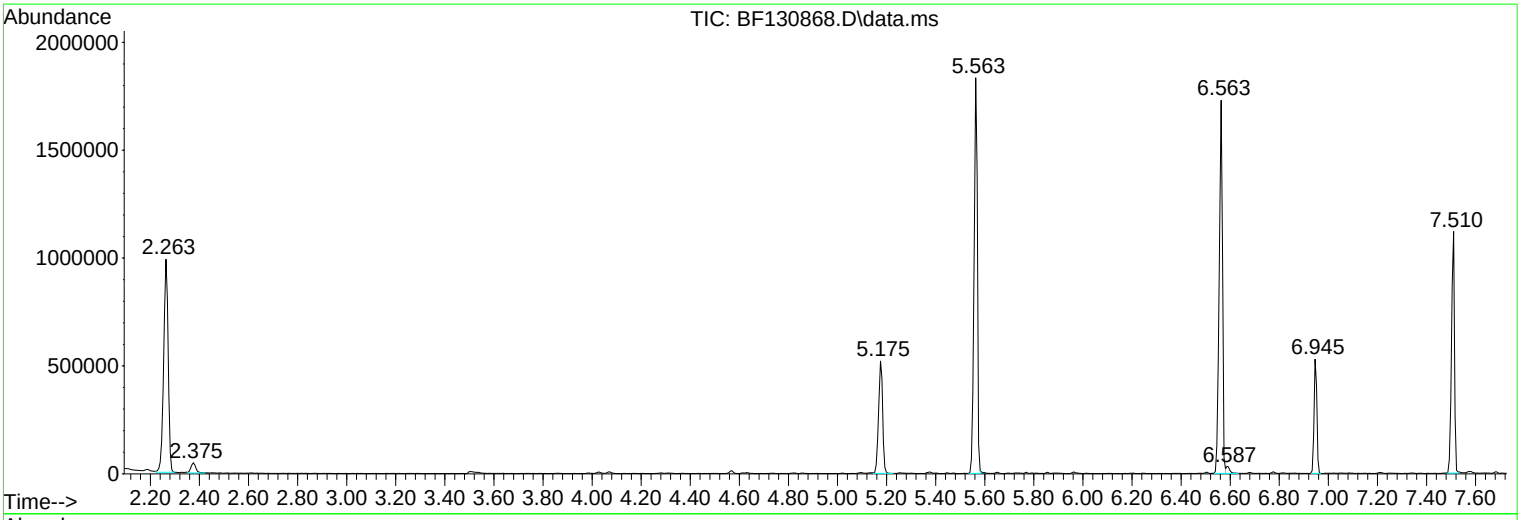
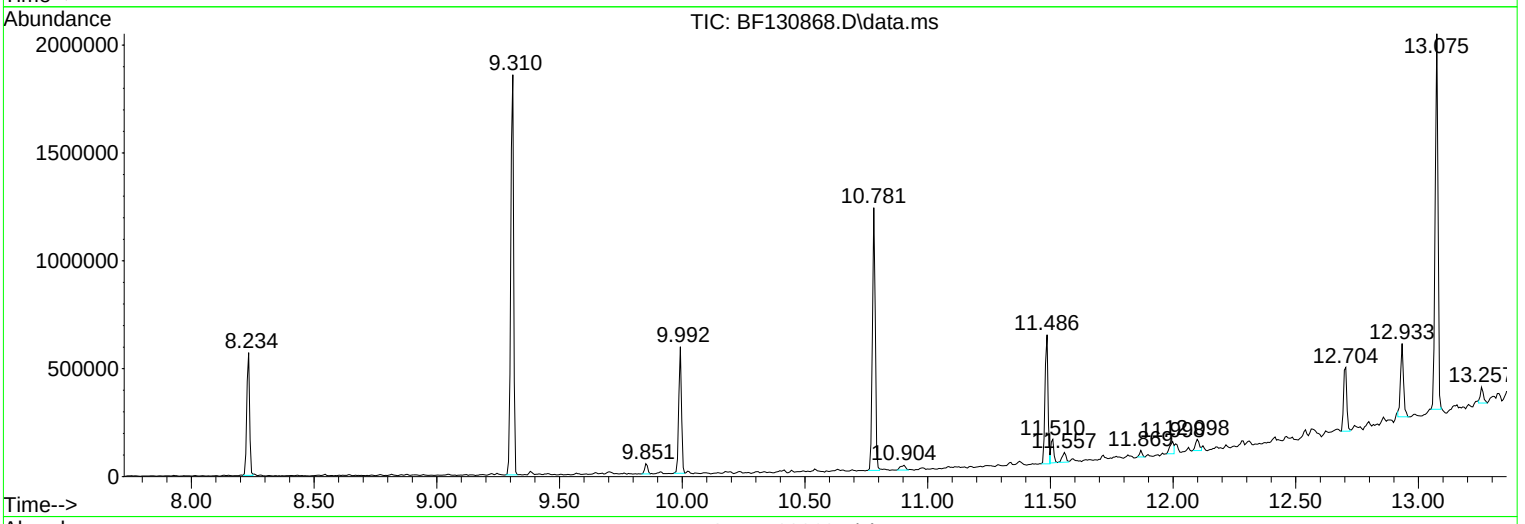
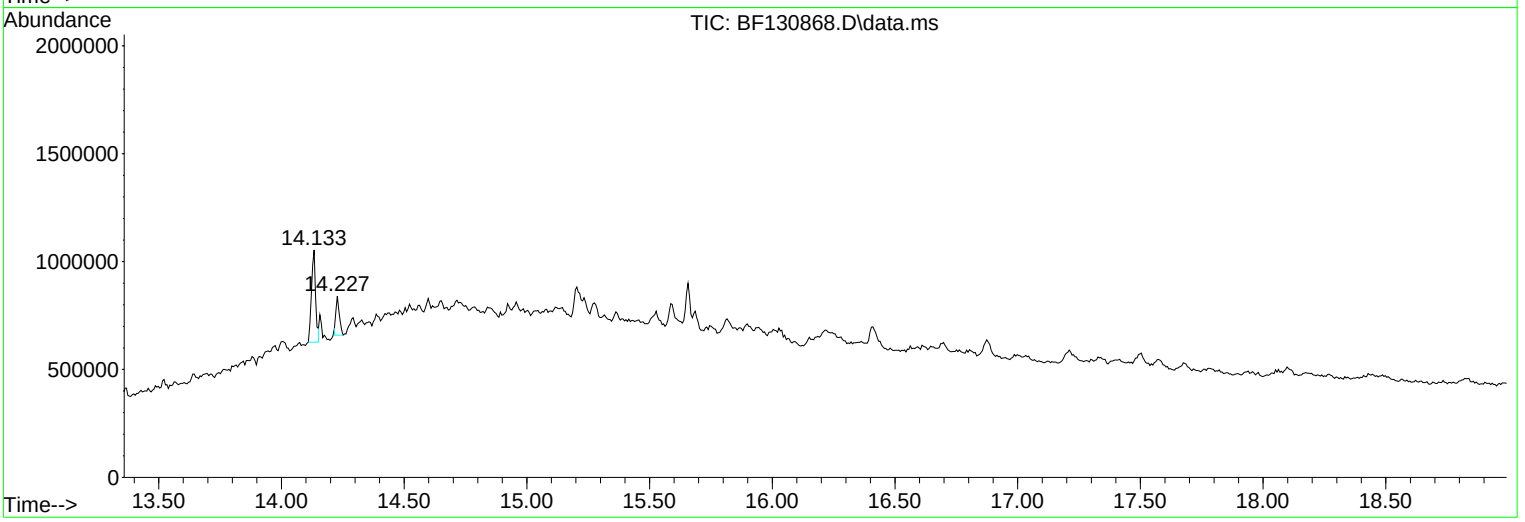
BNA_F
ClientSampleId :
CL-02-102622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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 Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

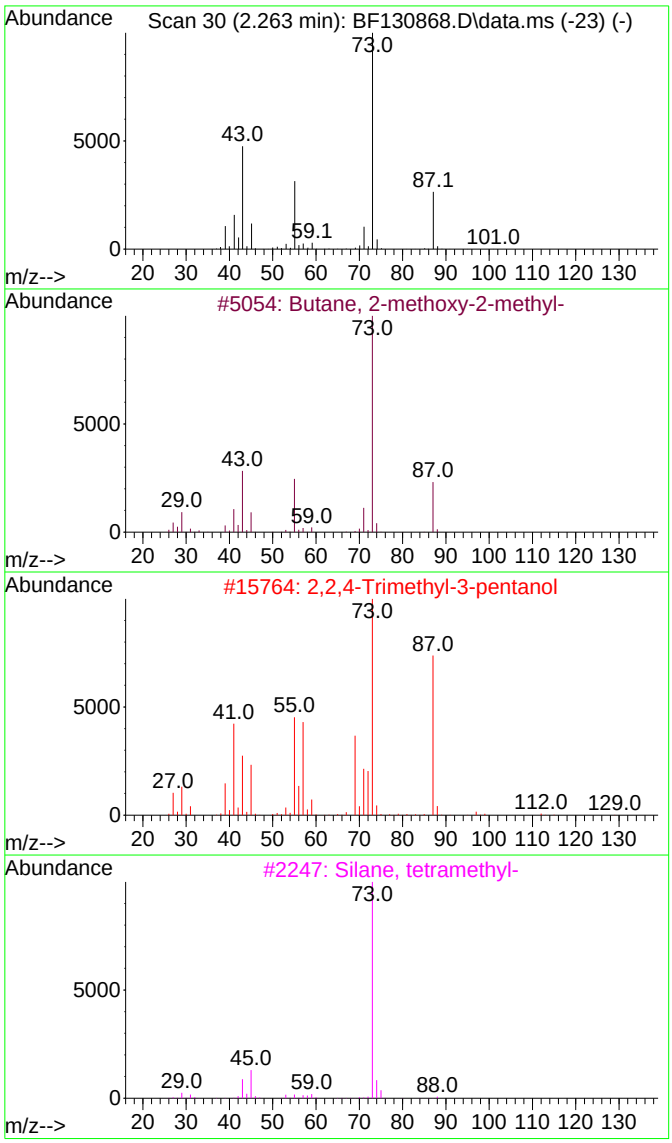
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

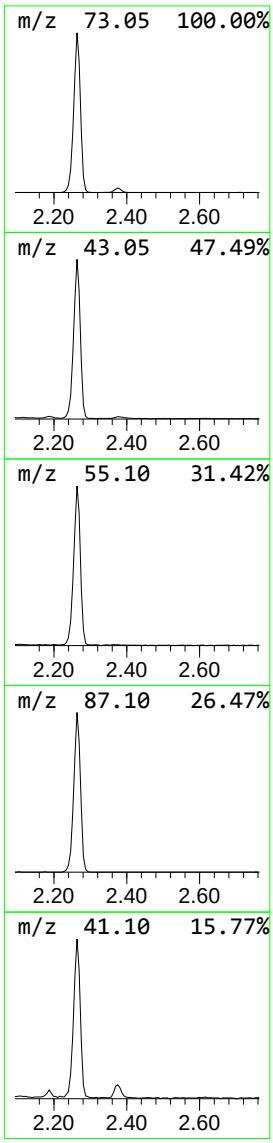
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	60.09 ng	1266310	1,4-Dichlorobenzene-d4	6.945

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





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Misc :
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Instrument :
BNA_F
ClientSampleId :
CL-02-102622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

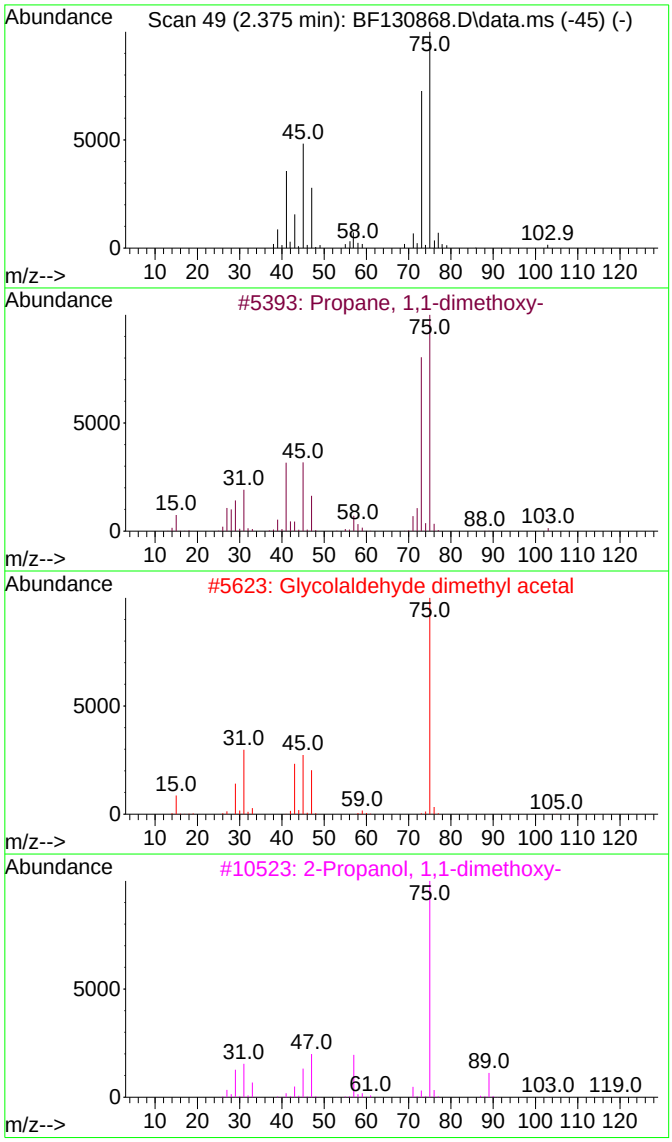
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

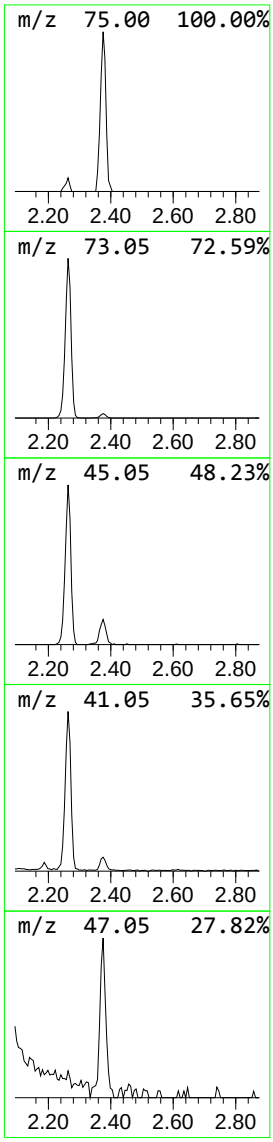
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.375	3.02 ng	63595	1,4-Dichlorobenzene-d4	6.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	59
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	56
3	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	53
4	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	42
5	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33





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Acq On : 29 Oct 2022 20:50
Operator : CG\JU
Sample : N5307-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-102622

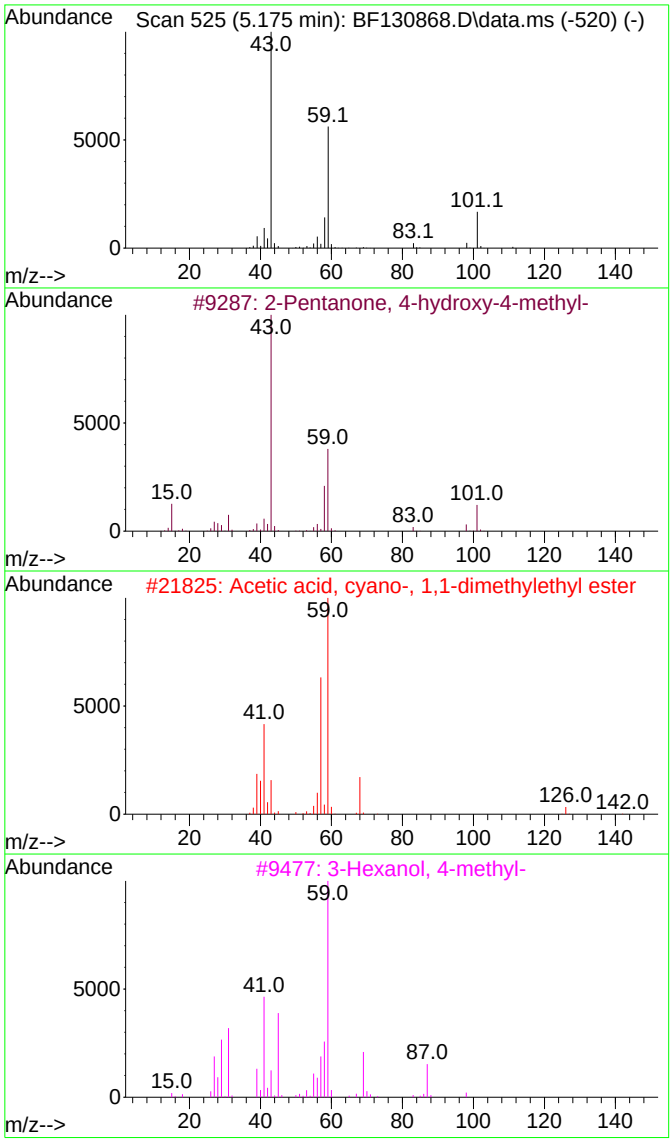
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

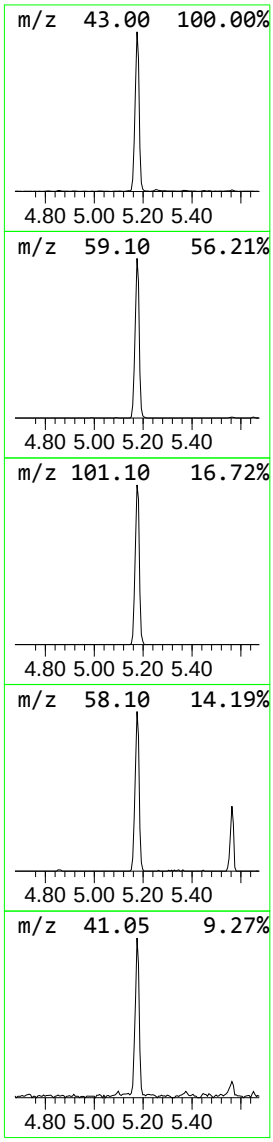
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	28.48 ng	600222	1,4-Dichlorobenzene-d4	6.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Operator : CG\JU
Sample : N5307-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-102622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

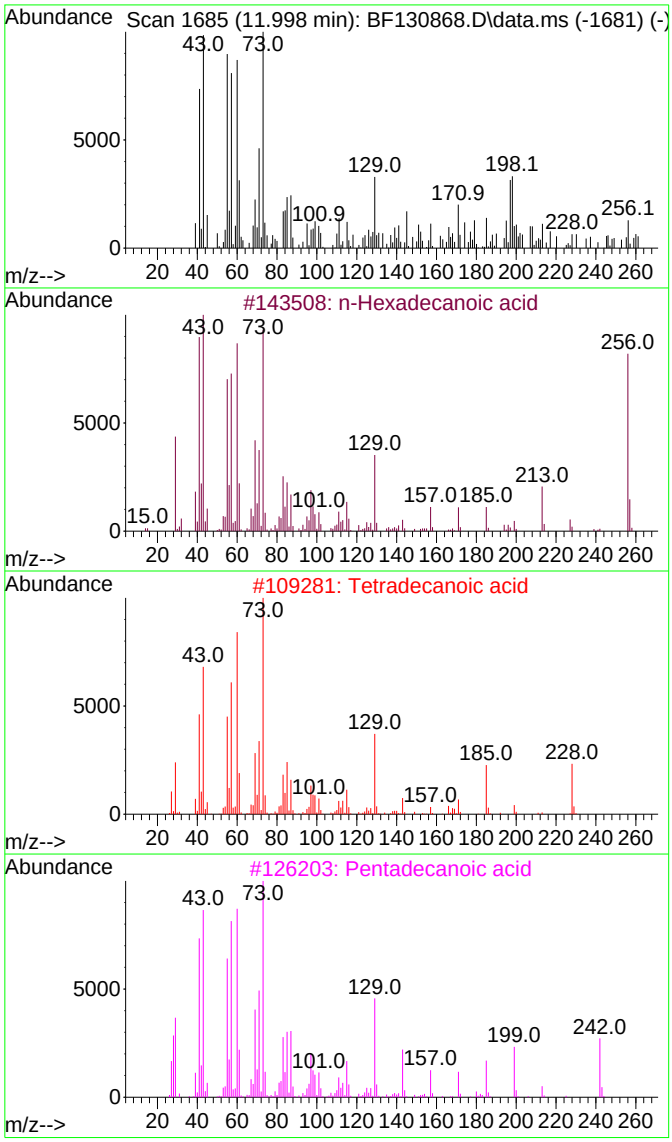
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

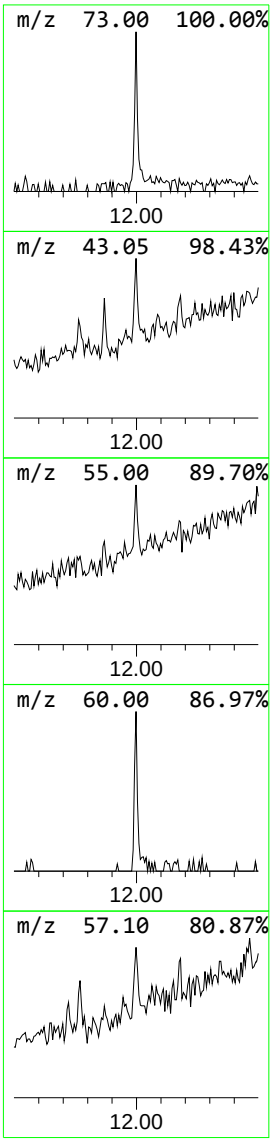
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	2.66 ng	65754	Phenanthrene-d10	11.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
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Misc :
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Instrument :
BNA_F
ClientSampleId :
CL-02-102622

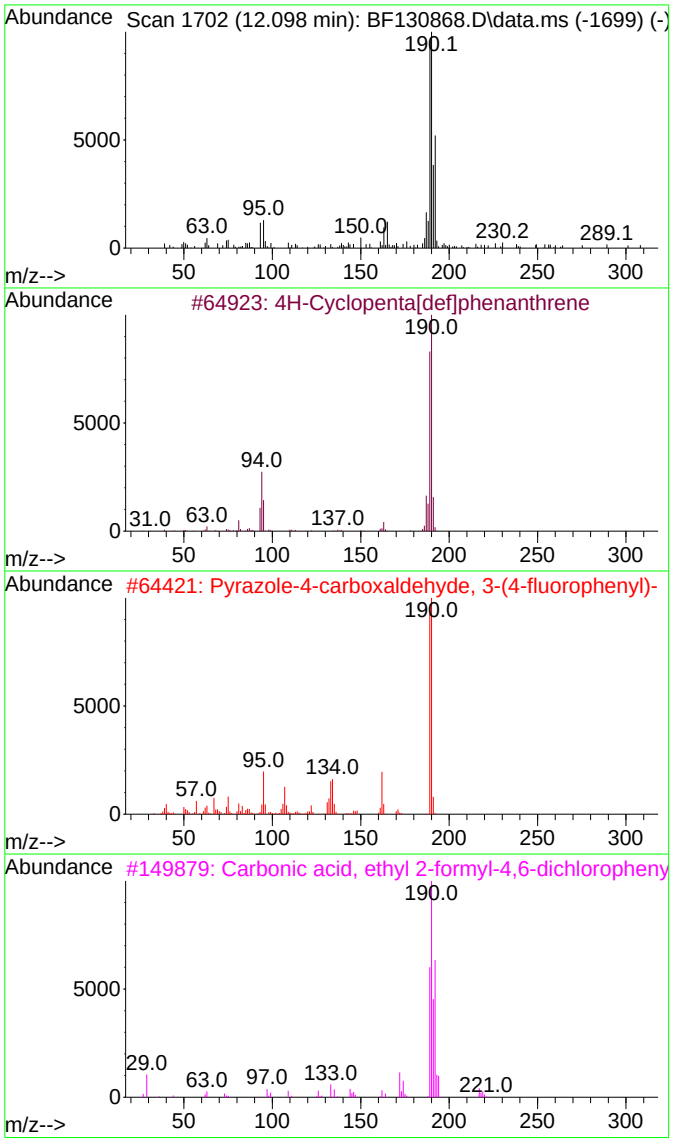
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

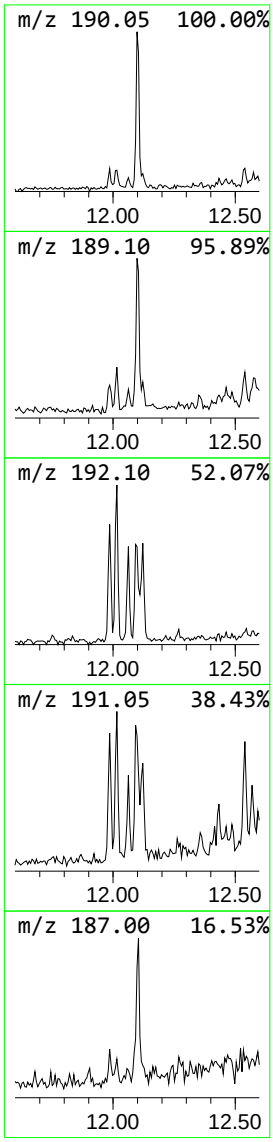
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.098	2.39 ng	59034	Phenanthrene-d10	11.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	47
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
4	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	35
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	30





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Misc :
ALS Vial : 19 Sample Multiplier: 1

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BNA_F
ClientSampleId :
CL-02-102622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

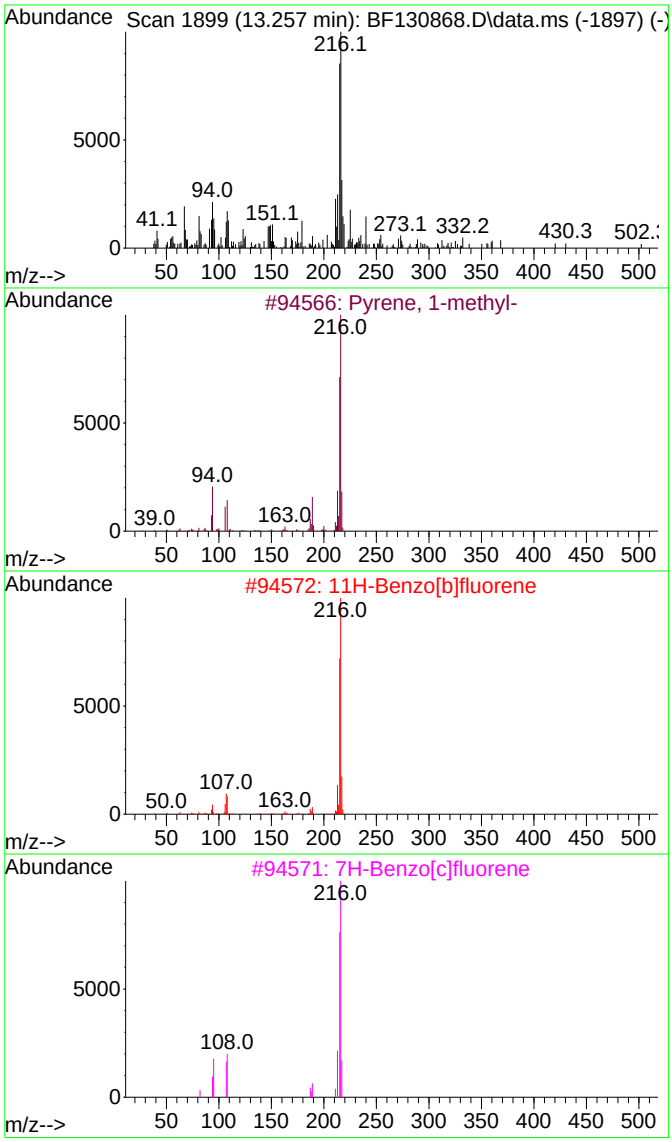
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

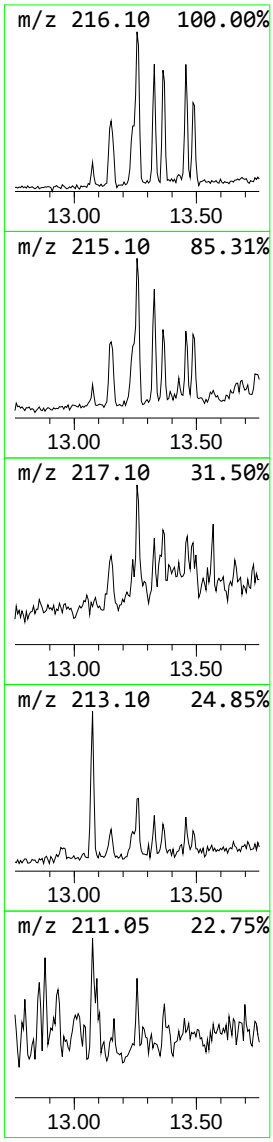
****

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.257	2.54 ng	63782	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	64
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	58
3	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	52
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	52
5	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	50





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Sample : N5307-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-102622

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

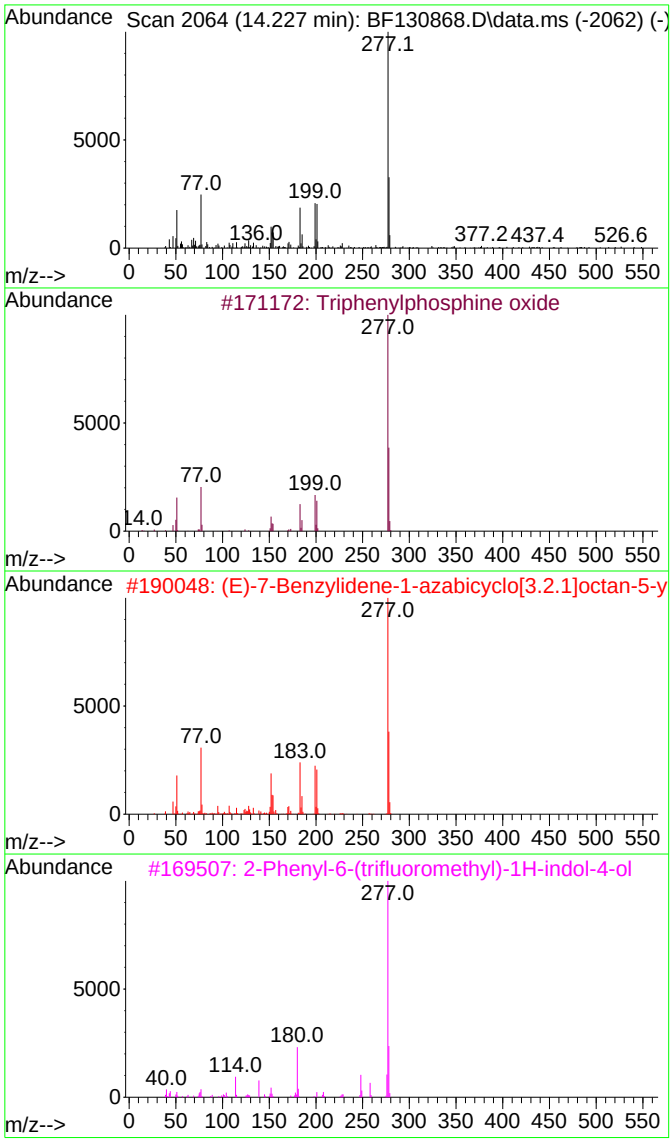
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

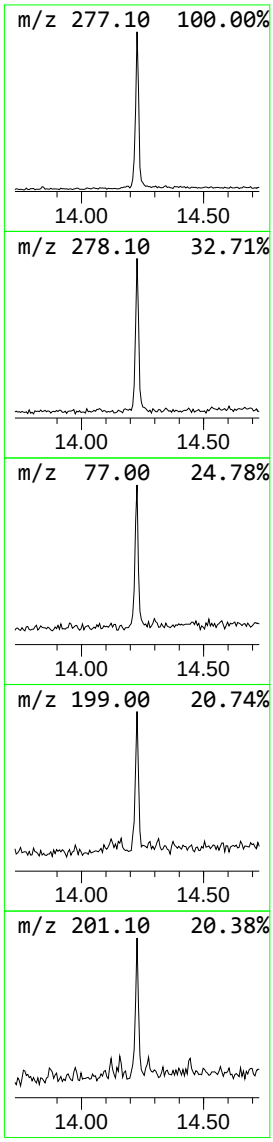
****

Peak Number 7 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.227	7.01 ng	176122	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	43
3	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	40
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	37
5	Benzoic acid, 2-(diphenylphosphi...	306	C19H15O2P	017261-28-8	33





Tentatively Identified Compound (LSC) summary

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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...	2.263	60.1	ng	1266310	1	6.945	421448	20.0
Propane, 1,1-di...	2.375	3.0	ng	63595	1	6.945	421448	20.0
2-Pentanone, 4-...	5.175	28.5	ng	600222	1	6.945	421448	20.0
n-Hexadecanoic ...	11.998	2.7	ng	65754	4	11.486	494316	20.0
4H-Cyclopenta[d...	12.098	2.4	ng	59034	4	11.486	494316	20.0
Pyrene, 1-methyl-	13.257	2.5	ng	63782	5	14.133	502258	20.0
Triphenylphosph...	14.227	7.0	ng	176122	5	14.133	502258	20.0