LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001046.D
Acq On : 15 Nov 2019 18:25
Operator : JU
Sample : K5832-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 10-(4-6)

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_P\METHODS\8270-BP110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.334	36	42	52	rVB	508508	769046	7.78%	1.098%
2	5.740	616	621	639	rVB	568816	930170	9.41%	1.329%
3	6.310	707	718	722	rBV	4125502	5388051	54.53%	7.696%
4	7.822	966	975	984	rBV	3967327	6127013	62.00%	8.752%
5	8.010	1000	1007	1011	rBV	4857173	6185182	62.59%	8.835%
6	8.369	1062	1068	1073	rBV	1172432	1370451	13.87%	1.957%
7	8.610	1102	1109	1113	rBV	4273500	5096227	51.57%	7.279%
8	9.246	1209	1217	1221	rBV	2895126	3765967	38.11%	5.379%
9	10.393	1406	1412	1417	rBV	1483366	1722123	17.43%	2.460%
10	12.175	1706	1715	1719	rBV	6441132	8371600	84.72%	11.958%
11	12.834	1822	1827	1832	rVB	553308	625432	6.33%	0.893%
12	13.251	1892	1898	1905	rBV	1846850	2287255	23.15%	3.267%
13	14.551	2110	2119	2131	rBV	4555634	6428806	65.06%	9.183%
14	14.851	2166	2170	2172	rBV	108359	130626	1.32%	0.187%
15	14.881	2172	2175	2181	rVB	91460	127364	1.29%	0.182%
16	15.563	2287	2291	2295	rVB	109257	111669	1.13%	0.160%
17	15.645	2301	2305	2309	rBV	1992847	2334081	23.62%	3.334%
18	16.198	2396	2399	2403	rVB	103398	106702	1.08%	0.152%
19	16.528	2449	2455	2462	rBV3	331110	494541	5.00%	0.706%
20	17.322	2586	2590	2594	rVB	88707	99558	1.01%	0.142%
21	17.386	2596	2601	2605	rBV	195873	228872	2.32%	0.327%
22	17.616	2637	2640	2648	rBV	102226	149553	1.51%	0.214%
23	17.692	2648	2653	2657	rVB	231172	269404	2.73%	0.385%
24	17.927	2687	2693	2697	rBV	8393233	9881729	100.00%	14.115%
25	18.292	2750	2755	2758	rBV3	89961	129948	1.32%	0.186%
26	19.163	2899	2903	2916	rBV	401451	738250	7.47%	1.054%
27	19.286	2918	2924	2927	rVV	2056966	2488909	25.19%	3.555%
28	19.316	2927	2929	2933	rVB2	148650	156540	1.58%	0.224%
29	19.574	2969	2973	2976	rBV	135883	142999	1.45%	0.204%
30	19.963	3036	3039	3042	rBV	141086	141576	1.43%	0.202%
31	20.339	3100	3103	3109	rVB2	150047	166104	1.68%	0.237%
32	20.569	3138	3142	3146	rBV	131162	220497	2.23%	0.315%
33	20.739	3167	3171	3175	rBV	149689	194952	1.97%	0.278%
34	20.916	3198	3201	3209	rVB	80329	102963	1.04%	0.147%

LSC Area Percent Report

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Acq On : 15 Nov 2019 18:25
Operator : JU
Sample : K5832-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 10-(4-6)

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_P\METHODS\8270-BP110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.063	3220	3226	3235	rVB	1552938	2207591	22.34%	3.153%
36	21.180	3243	3246	3252	rVB	121583	176712	1.79%	0.252%
37	21.686	3329	3332	3339	rVB	91375	142318	1.44%	0.203%

Sum of corrected areas: 70010781

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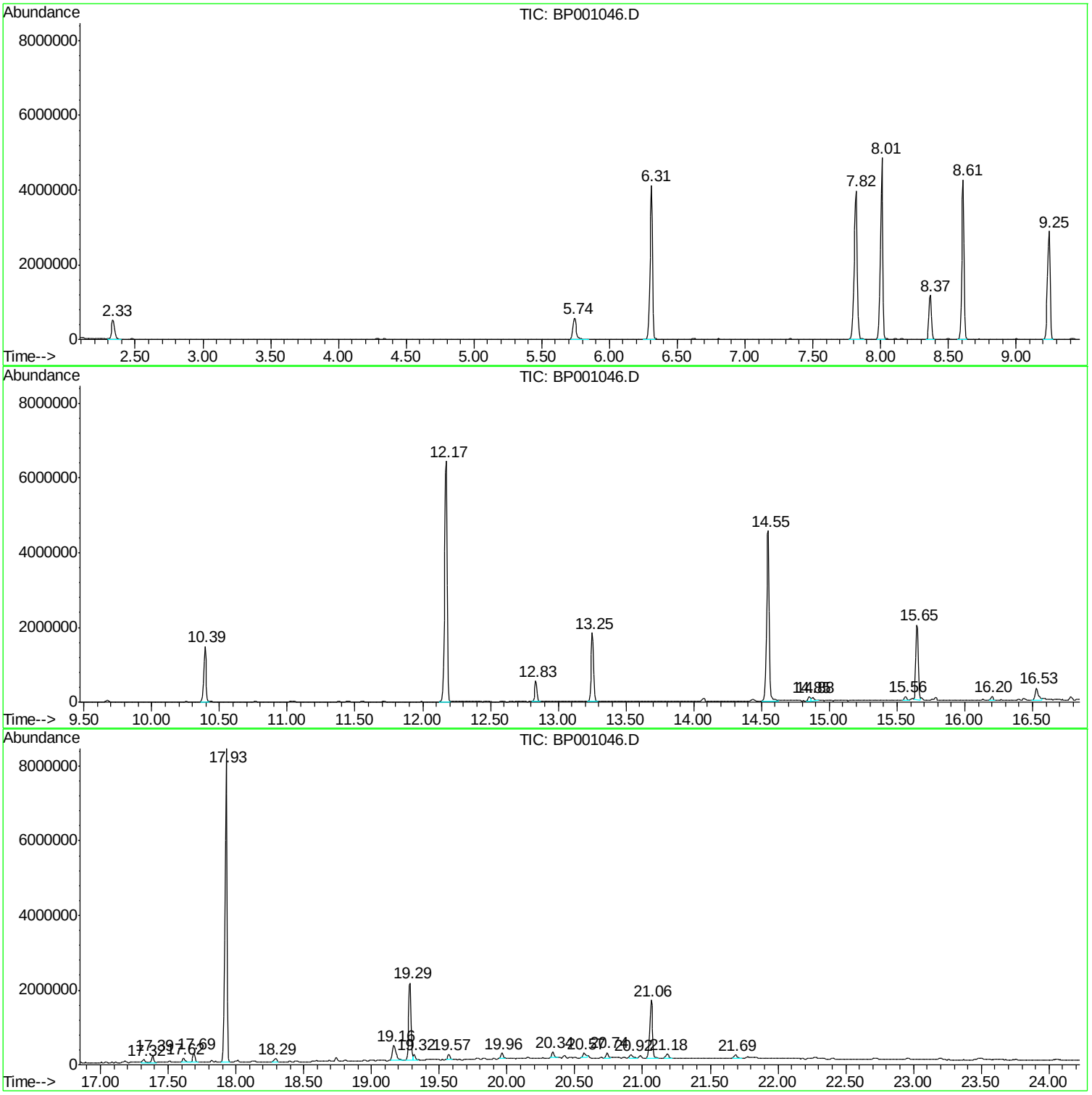
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
10-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001046.D
Acq On : 15 Nov 2019 18:25
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 10-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

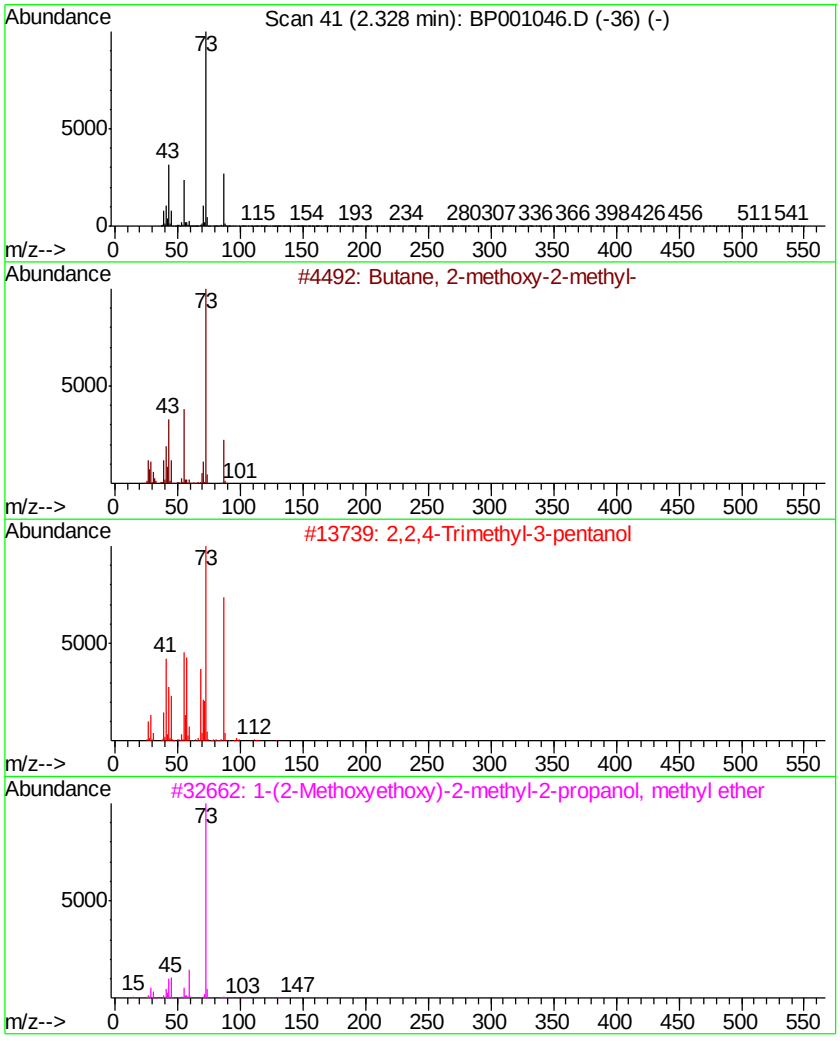
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

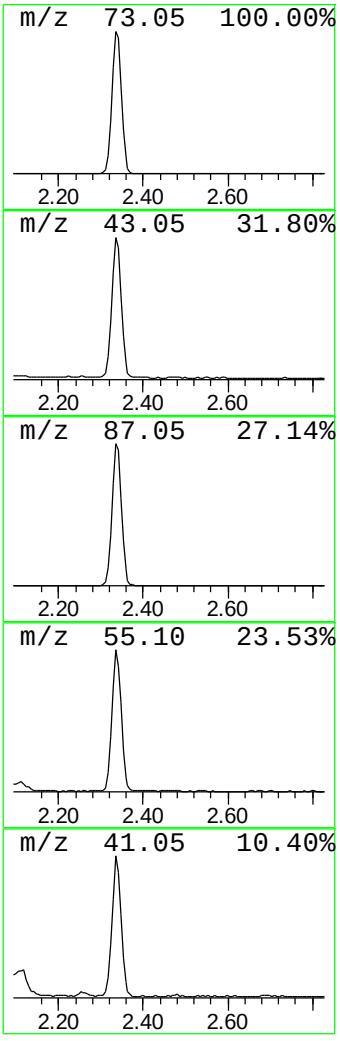
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	11.22 ng	769046	1,4-Dichlorobenzene-d4	8.37

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	39
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001046.D
Acq On : 15 Nov 2019 18:25
Operator : JU
Sample : K5832-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 10-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

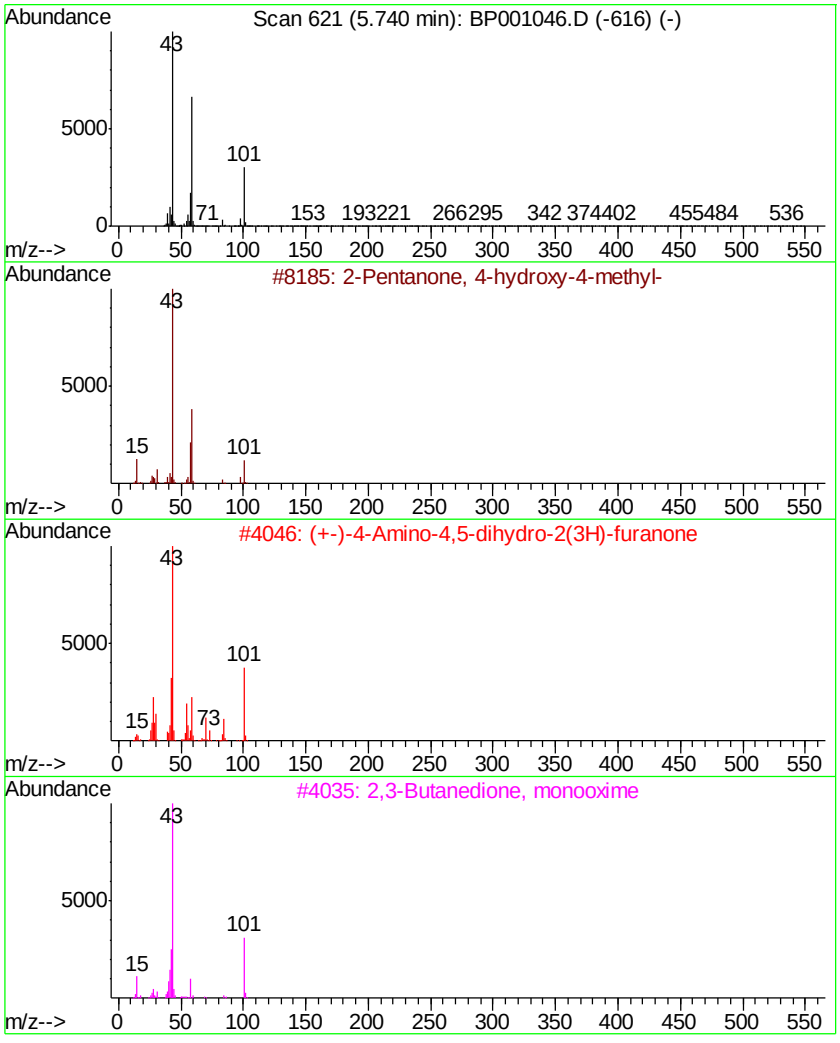
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

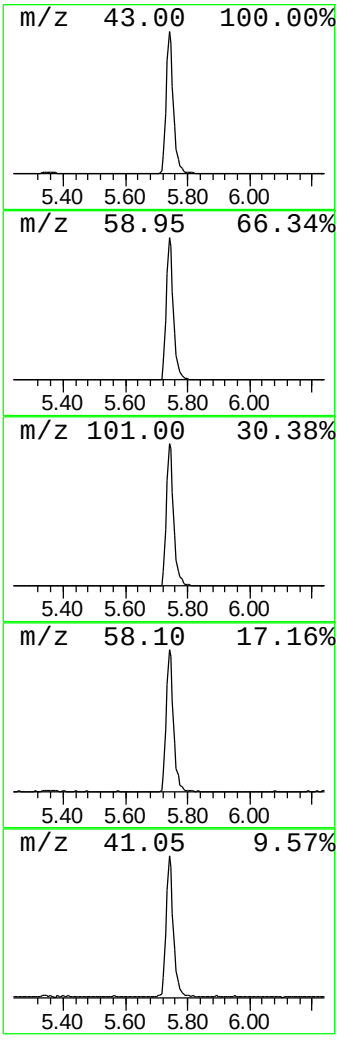
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.74	13.57 ng	930170	1,4-Dichlorobenzene-d4	8.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
5	2-Nonanone	142	C9H18O	000821-55-6	12





Library Search Compound Report

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Sample : K5832-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 10-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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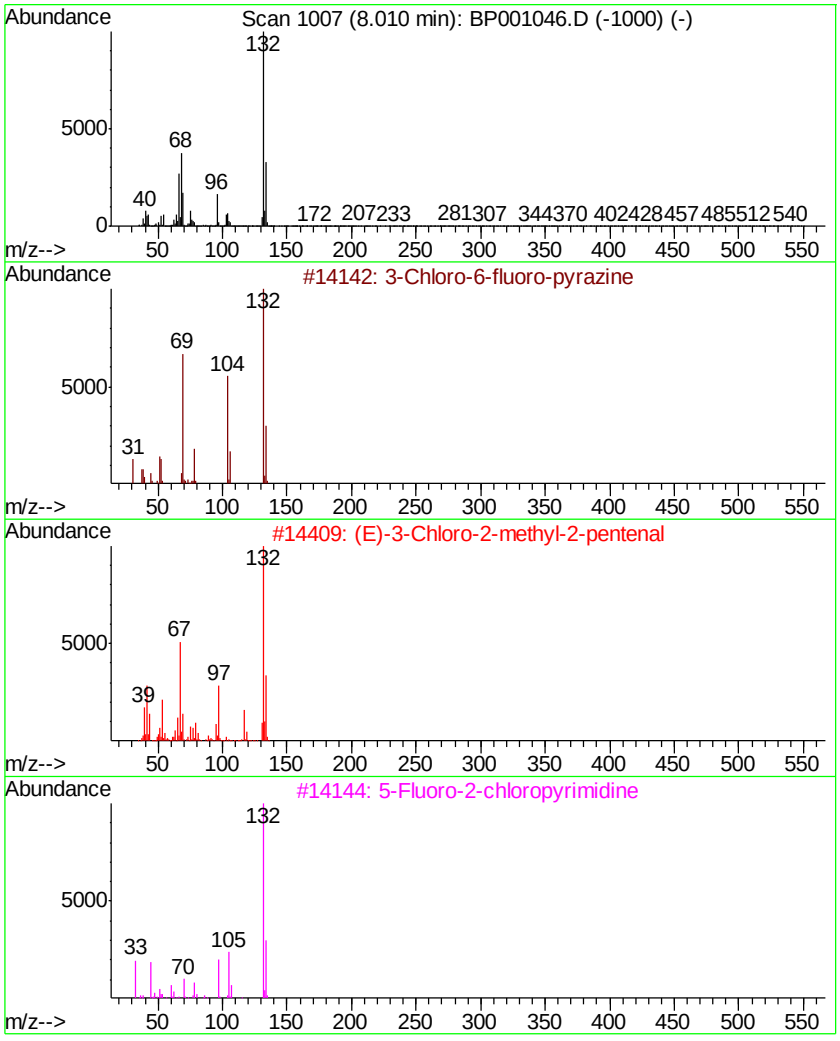
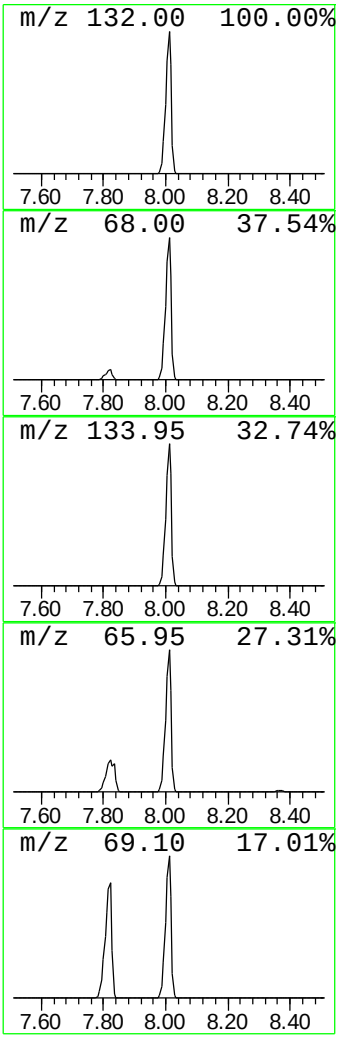
Peak Number 3 unknown8.01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	90.26 ng	6185180	1,4-Dichlorobenzene-d4	8.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
4	5-Aminoindole	132	C8H8N2	005192-03-0	16
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
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Operator : JU
Sample : K5832-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 10-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
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TIC Library : C:\DATABASE\NIST11.L
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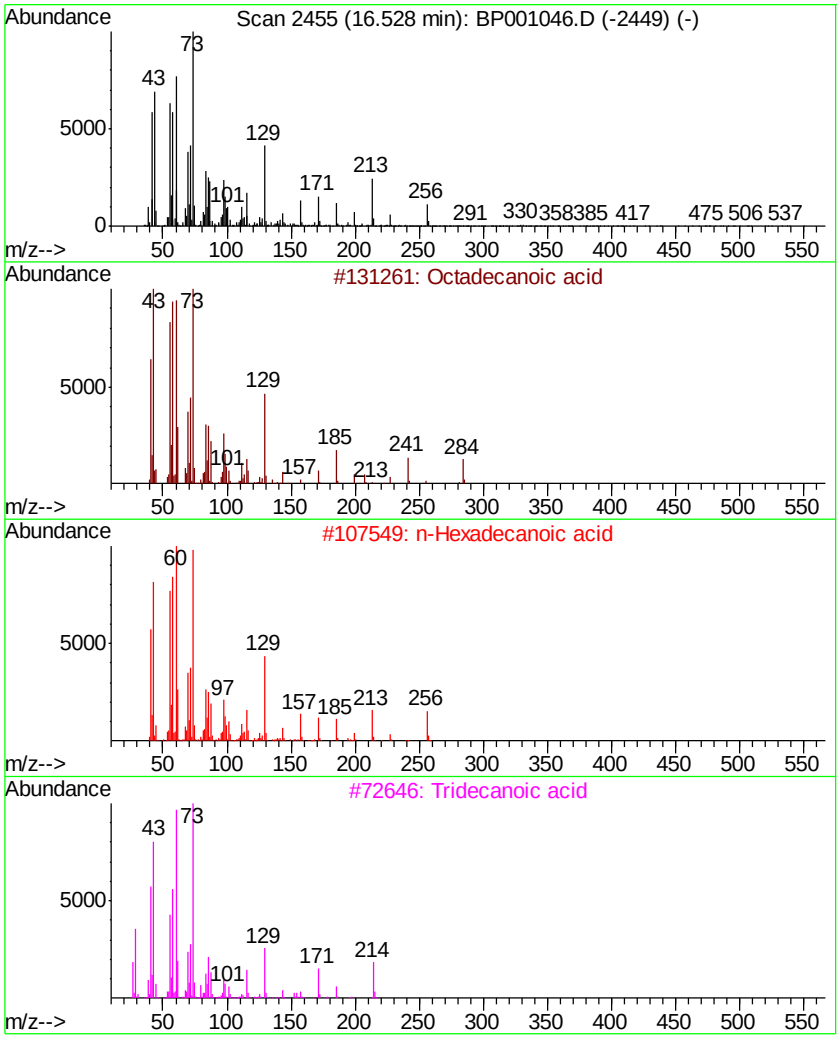
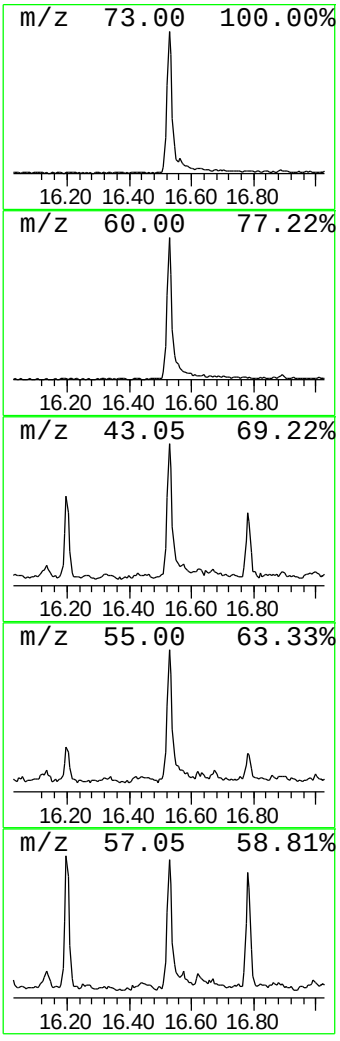
Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	4.24 ng	494541	Phenanthrene-d10	15.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	74





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Misc :
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Instrument : BNA_P
ClientSampleId : 10-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

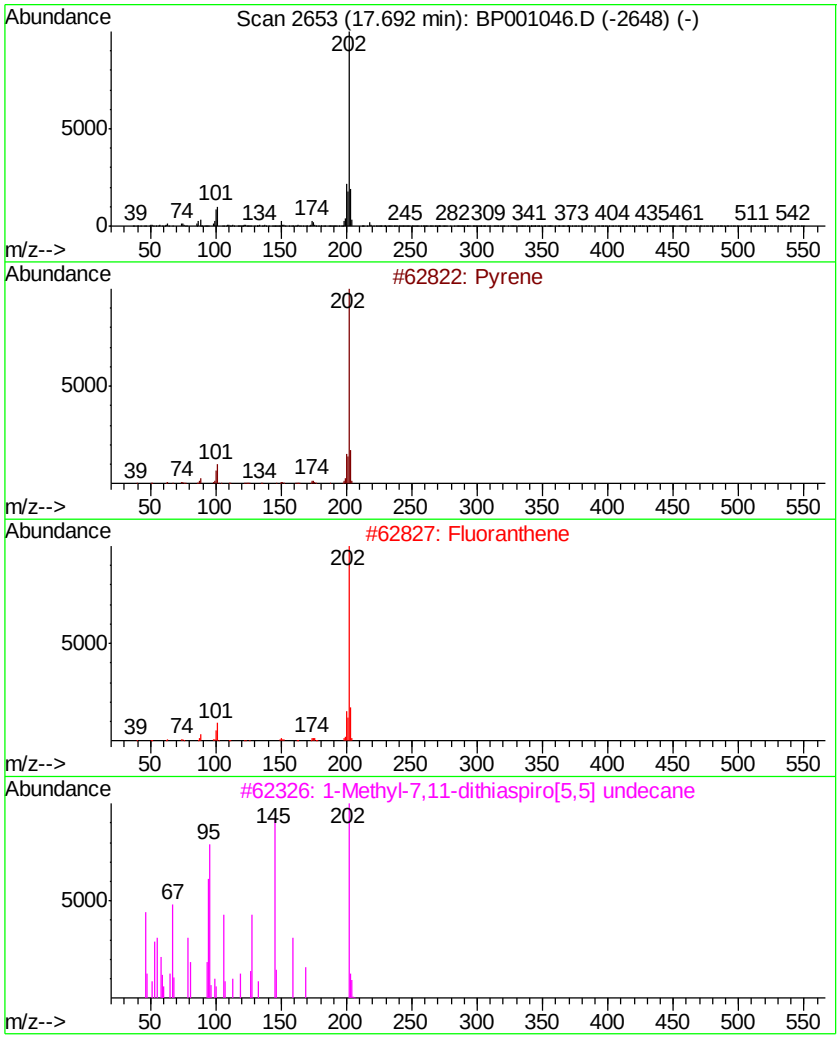
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

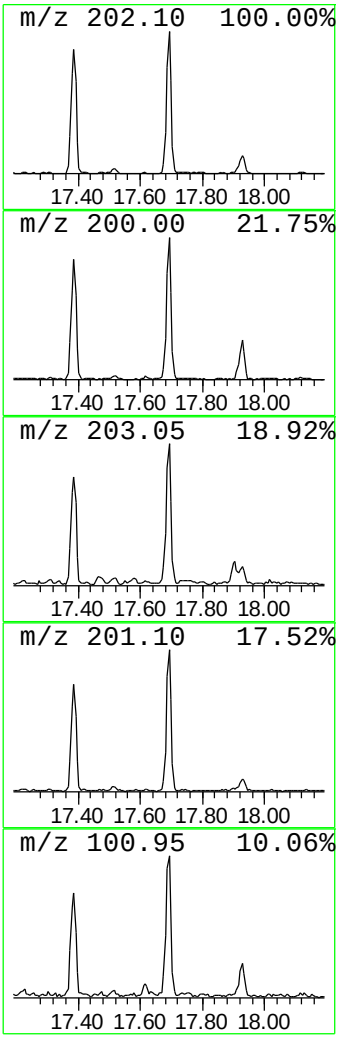
****

Peak Number 6 unknown17.69 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.69	2.16 ng	269404	Chrysene-d12	19.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	96
2	Fluoranthene	202	C16H10	000206-44-0	81
3	1-Methyl-7,11-dithiaspiro[5,5] u...	202	C10H18S2	107678-22-8	47
4	Benzaldehyde, 2,6-difuloro-3,4-d...	202	C9H8F2O3	152434-99-6	9
5	Pyrimidine, 4-methoxy-6-(2-hydro...	202	C11H10N2O2	097630-79-0	9





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ClientSampleId : 10-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

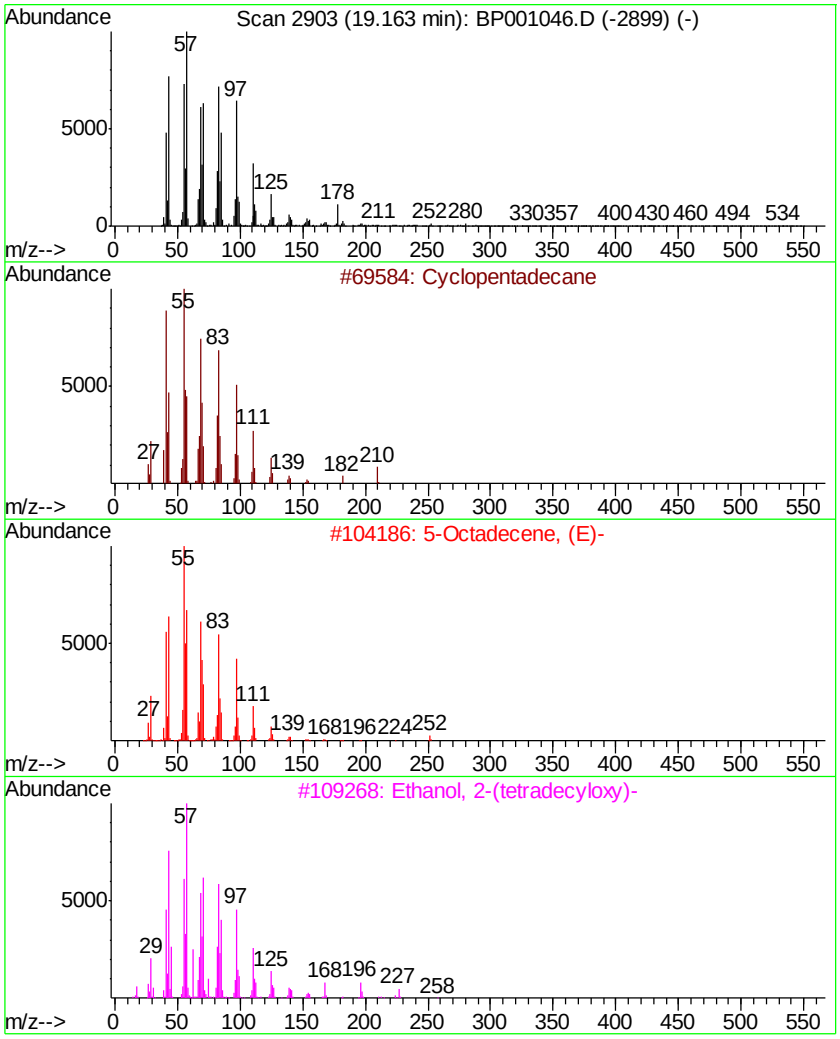
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

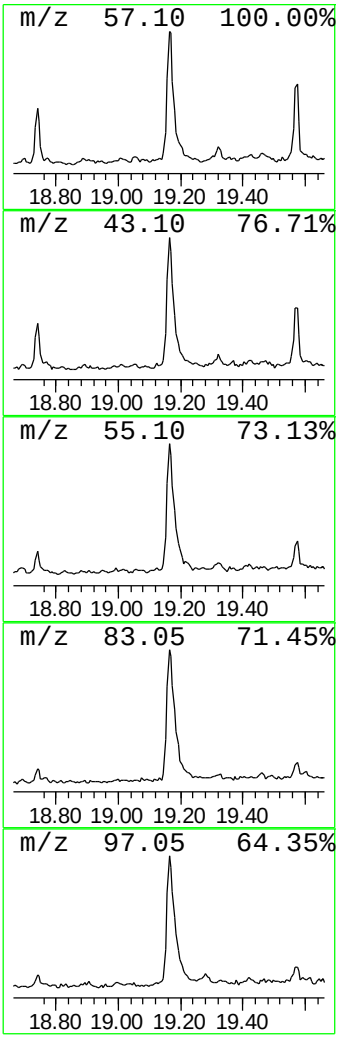
****

Peak Number 7 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.16	5.93 ng	738250	Chrysene-d12	19.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	96
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	94
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	89
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.33	11.2	ng	769046	1	8.37	1370450	20.0
2-Pentanone, 4-hy...	5.74	13.6	ng	930170	1	8.37	1370450	20.0
unknown8.01	8.01	90.3	ng	6185180	1	8.37	1370450	20.0
Octadecanoic acid	16.53	4.2	ng	494541	4	15.65	2334080	20.0
unknown17.69	17.69	2.2	ng	269404	5	19.29	2488910	20.0
Cyclopentadecane	19.16	5.9	ng	738250	5	19.29	2488910	20.0