LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112020\
Data File : BP004024.D
Acq On : 20 Nov 2020 14:41
Operator : CG/JU
Sample : L4808-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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-BP110320.M
Title : D

Signal : TIC: BP004024.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.922	3	6	25	rVB	4408103	5580635	100.00%	16.010%
2	3.075	26	32	43	rBV	79853	169597	3.04%	0.487%
3	3.169	43	48	56	rVB	253532	341498	6.12%	0.980%
4	3.969	179	184	190	rVB	44922	62745	1.12%	0.180%
5	4.628	290	296	310	rBV	2353173	3295842	59.06%	9.455%
6	5.269	398	405	418	rBV	1895558	2703054	48.44%	7.755%
7	5.805	488	496	508	rBV	390199	610755	10.94%	1.752%
8	7.446	766	775	787	rBV	1073977	1944162	34.84%	5.578%
9	8.269	906	915	922	rBV	449211	729668	13.07%	2.093%
10	9.428	1102	1112	1121	rBV	1101617	1828349	32.76%	5.245%
11	11.098	1387	1396	1410	rBV	574405	984855	17.65%	2.825%
12	12.704	1663	1669	1674	rBV	42684	62317	1.12%	0.179%
13	13.510	1799	1806	1819	rBV	2599409	3649636	65.40%	10.470%
14	13.710	1835	1840	1847	rBV3	47008	78985	1.42%	0.227%
15	14.310	1938	1942	1949	rBV	75050	112825	2.02%	0.324%
16	14.886	2030	2040	2047	rBV	875249	1367008	24.50%	3.922%
17	15.663	2167	2172	2177	rBV	32211	55998	1.00%	0.161%
18	15.928	2212	2217	2226	rVB2	40135	61582	1.10%	0.177%
19	16.375	2288	2293	2300	rBV2	107829	176649	3.17%	0.507%
20	17.622	2499	2505	2509	rBV	1049717	1473505	26.40%	4.227%
21	17.663	2509	2512	2520	rVV	215480	299570	5.37%	0.859%
22	17.751	2523	2527	2532	rVB	63713	86106	1.54%	0.247%

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Misc :
ALS Vial : 8 Sample Multiplier: 1

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

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Title : D

23	18.522	2653	2658	2662	rBV2	50347	79775	1.43%	0.229%
24	18.663	2676	2682	2685	rBV4	58462	95018	1.70%	0.273%
25	19.174	2766	2769	2772	rBV2	58143	75758	1.36%	0.217%
26	19.210	2772	2775	2781	rVV2	57426	89466	1.60%	0.257%
27	19.333	2794	2796	2801	rBV5	42814	63089	1.13%	0.181%
28	19.598	2836	2841	2846	rBV	283453	384338	6.89%	1.103%
29	19.945	2897	2900	2904	rVB	215468	275519	4.94%	0.790%
30	20.051	2915	2918	2923	rBV3	103648	190606	3.42%	0.547%
31	20.121	2925	2930	2936	rVB	4055648	4904950	87.89%	14.072%
32	20.827	3047	3050	3052	rBV2	108216	113378	2.03%	0.325%
33	21.657	3186	3191	3195	rVB	1087975	1544071	27.67%	4.430%
34	24.127	3606	3611	3618	rVB	702782	1365498	24.47%	3.917%

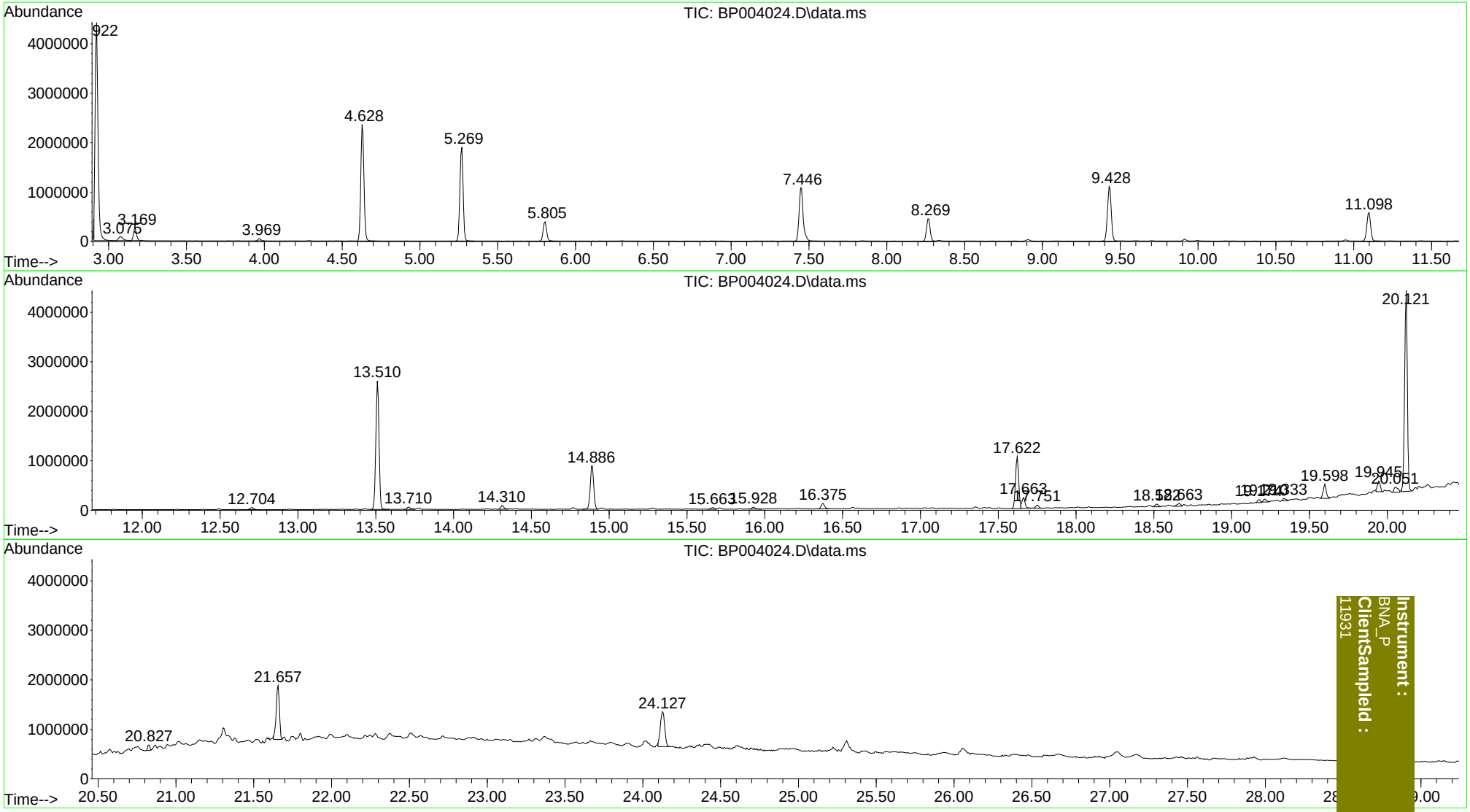
Sum of corrected areas: 34856807

Instrument :
BNA_P
ClientSampleId :
11931

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112020\
Data File : BP004024.D
Acq On : 20 Nov 2020 14:41
Operator : CG/JU
Sample : L4808-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112020\
Data File : BP004024.D
Acq On : 20 Nov 2020 14:41
Operator : CG/JU
Sample : L4808-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.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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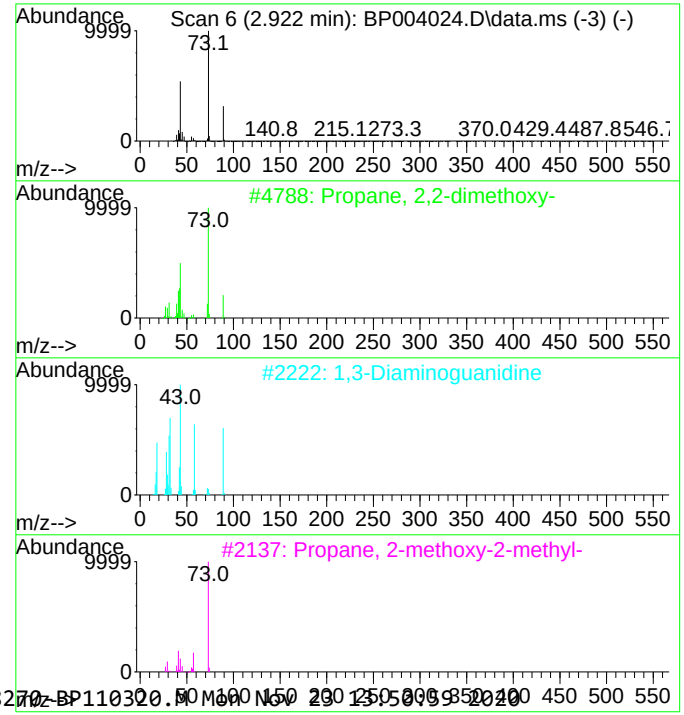
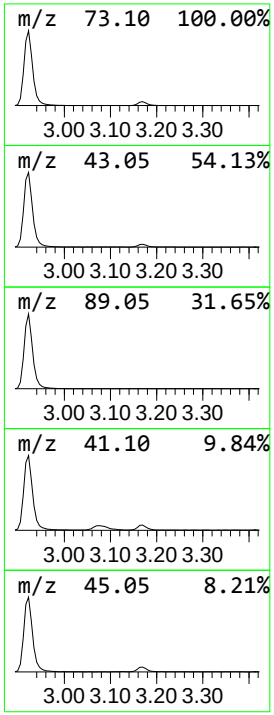
Peak Number 1 unknown2.92 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.922	152.96 ng	5580640	1,4-Dichlorobenzene-d4	8.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9





Instrument :
BNA_P
ClientSampleId :
11931

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112020\
Data File : BP004024.D
Acq On : 20 Nov 2020 14:41
Operator : CG/JU
Sample : L4808-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.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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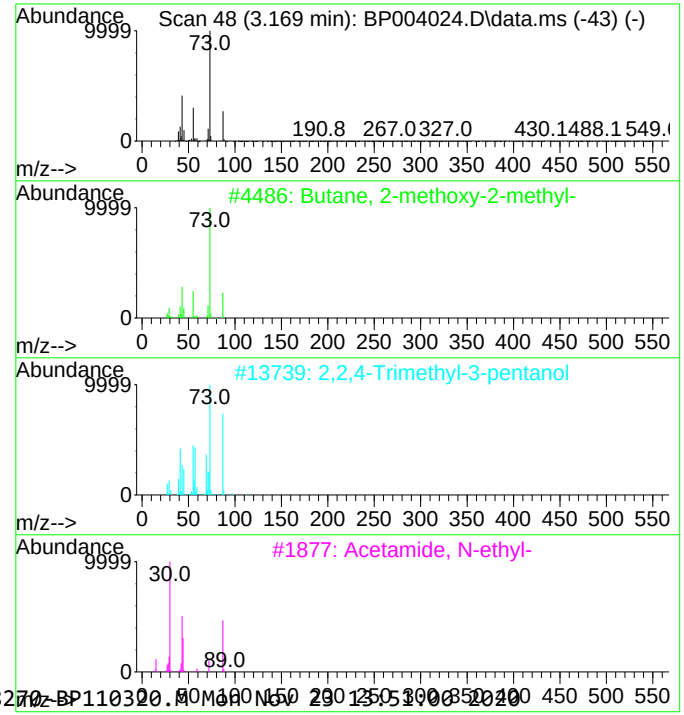
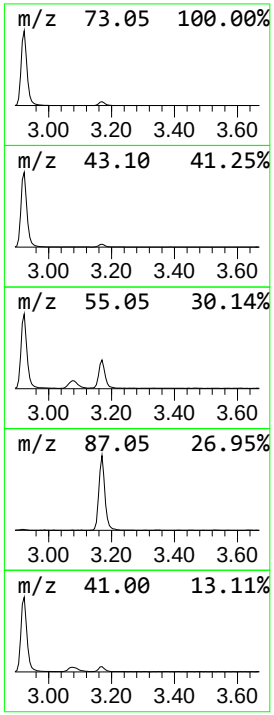
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.169	9.36 ng	341498	1,4-Dichlorobenzene-d4	8.269

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Instrument :
BNA_P
ClientSampleId :
11931

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112020\
Data File : BP004024.D
Acq On : 20 Nov 2020 14:41
Operator : CG/JU
Sample : L4808-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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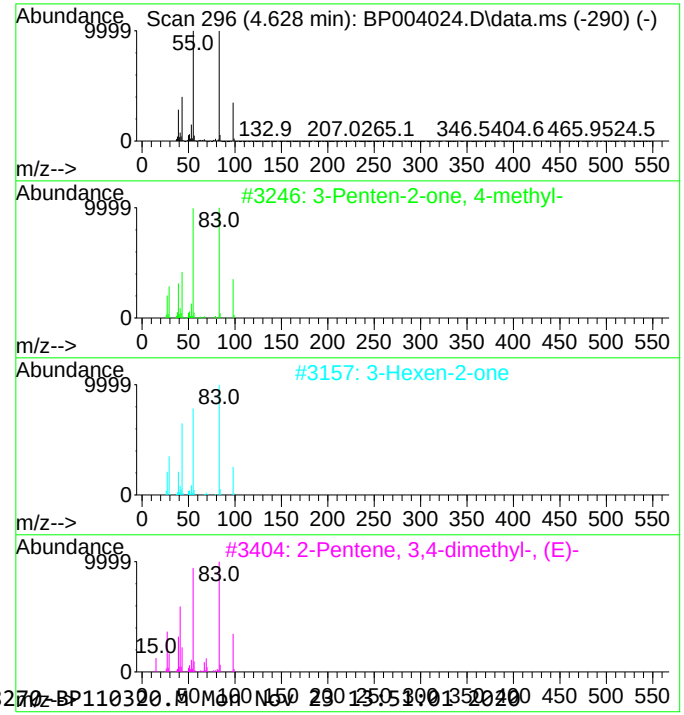
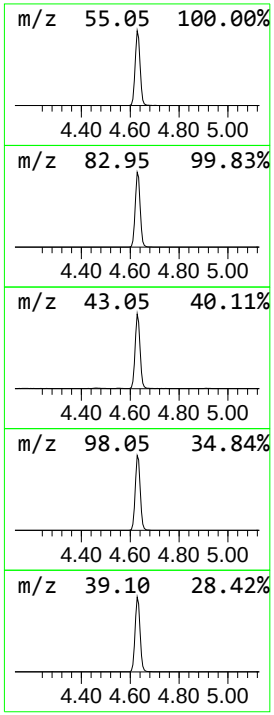
Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.628	90.34 ng	3295840	1,4-Dichlorobenzene-d4	8.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Instrument :
BNA_P
ClientSampleId :
11931

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112020\
Data File : BP004024.D
Acq On : 20 Nov 2020 14:41
Operator : CG/JU
Sample : L4808-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

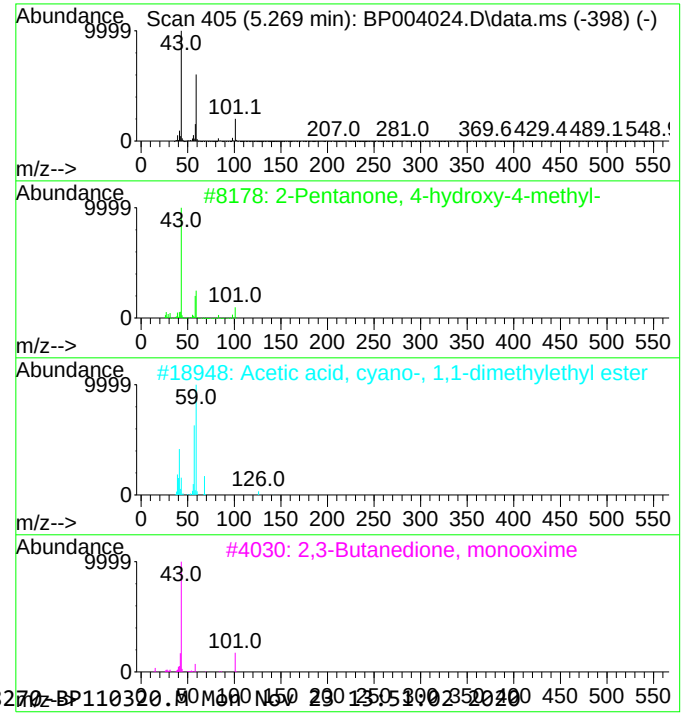
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

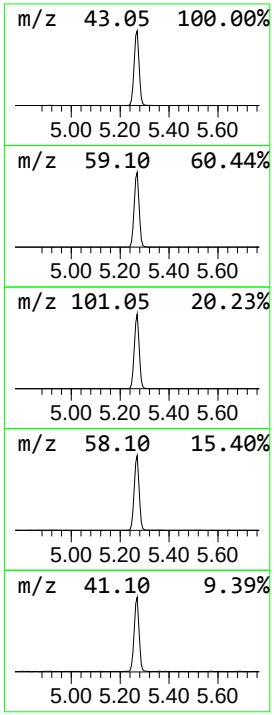
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.269	74.09 ng	2703050	1,4-Dichlorobenzene-d4	8.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Instrument :
BNA_P
ClientSampleId :
11931

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112020\
Data File : BP004024.D
Acq On : 20 Nov 2020 14:41
Operator : CG/JU
Sample : L4808-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.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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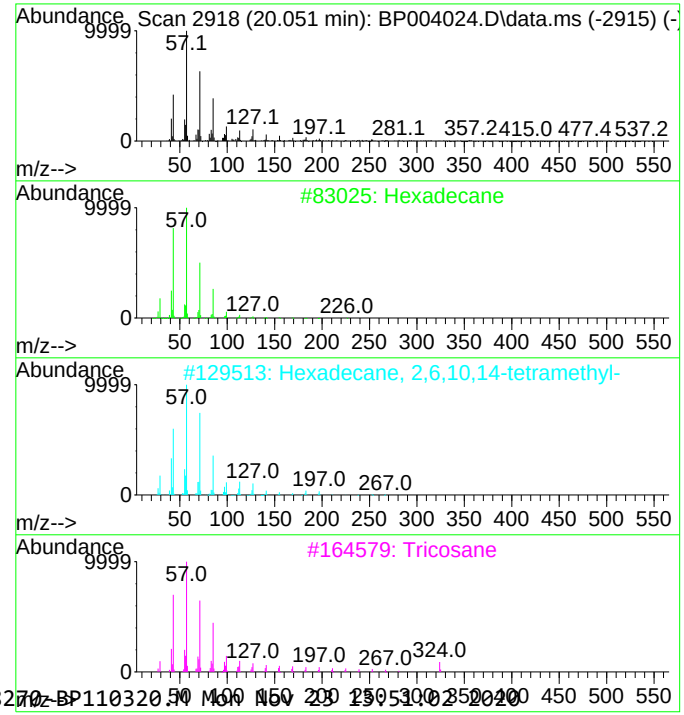
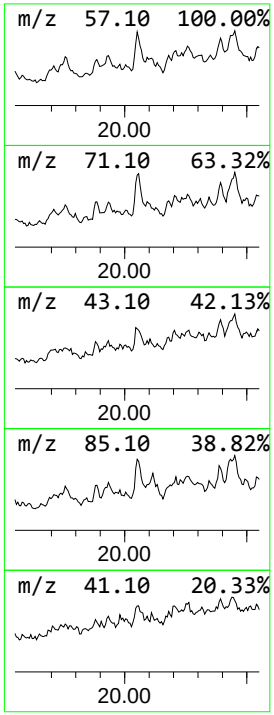
Peak Number 6 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.051	2.47 ng	190606	Chrysene-d12	21.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	94
3	Tricosane	324	C23H48	000638-67-5	93
4	Nonadecane	268	C19H40	000629-92-5	93
5	Docosane	310	C22H46	000629-97-0	90





Instrument :
BNA_P
ClientSampleId :
11931

Tentatively Identified Compound (LSC) summary

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Misc :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
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
unknown2.92	2.922	153.0	ng	5580640	1	8.269	729668	20.0
Butane, 2-metho...	3.169	9.4	ng	341498	1	8.269	729668	20.0
3-Penten-2-one,...	4.628	90.3	ng	3295840	1	8.269	729668	20.0
2-Pentanone, 4-...	5.269	74.1	ng	2703050	1	8.269	729668	20.0
Hexadecane	20.051	2.5	ng	190606	5	21.657	1544070	20.0

Instrument :
BNA_P
ClientSampleId :
11931