LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP112719\
Data File : BP001101.D
Acq On : 28 Nov 2019 01:36
Operator : JU
Sample : K5977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WS-112119-0-2-COMP-B1

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-BP112719.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	4.781	453	458	471	rBV	723648	1108108	25.92%	2.668%
2	5.640	598	604	617	rBV	1271971	1774572	41.51%	4.273%
3	6.228	698	704	720	rVB	1246136	1503742	35.17%	3.621%
4	7.769	959	966	982	rVB	2752122	3433335	80.31%	8.267%
5	7.957	993	998	1012	rVB	2035308	2599944	60.82%	6.260%
6	8.328	1055	1061	1068	rVB	885067	1043897	24.42%	2.514%
7	8.569	1096	1102	1107	rBV	2297323	2748580	64.29%	6.618%
8	9.204	1203	1210	1214	rBV	1954997	2283069	53.40%	5.497%
9	10.357	1401	1406	1411	rBV	1104777	1365982	31.95%	3.289%
10	12.145	1703	1710	1714	rBV	3308439	4191645	98.05%	10.093%
11	12.810	1813	1823	1829	rBV	577347	629983	14.74%	1.517%
12	13.228	1887	1894	1899	rBV	1292390	1606488	37.58%	3.868%
13	13.275	1899	1902	1907	rVB	43293	51751	1.21%	0.125%
14	14.122	2043	2046	2053	rVB	35845	45194	1.06%	0.109%
15	14.516	2106	2113	2124	rVB5	26451	59506	1.39%	0.143%
16	15.622	2292	2301	2304	rBV	1412985	1637393	38.30%	3.943%
17	15.657	2304	2307	2312	rVB	533692	555356	12.99%	1.337%
18	15.733	2317	2320	2323	rVV	79780	79352	1.86%	0.191%
19	16.381	2423	2430	2433	rBV	85215	107005	2.50%	0.258%
20	16.416	2433	2436	2444	rVB	128949	142513	3.33%	0.343%
21	16.528	2450	2455	2459	rVV	128956	171683	4.02%	0.413%
22	16.563	2459	2461	2466	rVB	65571	75015	1.75%	0.181%
23	16.816	2499	2504	2513	rVB2	73065	116289	2.72%	0.280%
24	17.163	2559	2563	2567	rBV2	61164	81218	1.90%	0.196%
25	17.369	2593	2598	2602	rBV	819260	872125	20.40%	2.100%
26	17.563	2626	2631	2637	rBV3	26941	48466	1.13%	0.117%
27	17.675	2644	2650	2654	rVB	838238	984850	23.04%	2.371%
28	17.751	2654	2663	2666	rBV2	27679	58664	1.37%	0.141%
29	17.845	2676	2679	2682	rBV	39387	42770	1.00%	0.103%
30	17.910	2682	2690	2694	rVV	3673461	4275062	100.00%	10.294%
31	17.986	2696	2703	2707	rBV3	53802	101201	2.37%	0.244%
32	18.098	2717	2722	2724	rBV4	49482	81942	1.92%	0.197%
33	18.127	2724	2727	2731	rVB	85229	101868	2.38%	0.245%
34	18.263	2746	2750	2761	rVV5	102519	187173	4.38%	0.451%

LSC Area Percent Report

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Acq On : 28 Nov 2019 01:36
Operator : JU
Sample : K5977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WS-112119-0-2-COMP-B1

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-BP112719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.380	2767	2770	2774	rVB2	60315	62281	1.46%	0.150%
36	18.422	2774	2777	2780	rBV	48823	56988	1.33%	0.137%
37	18.580	2801	2804	2809	rVB3	32236	42940	1.00%	0.103%
38	18.727	2826	2829	2835	rVB	52073	52500	1.23%	0.126%
39	18.786	2835	2839	2847	rVB	76233	103641	2.42%	0.250%
40	18.933	2860	2864	2869	rBV2	62518	103476	2.42%	0.249%
41	18.980	2869	2872	2874	rBV	56059	60105	1.41%	0.145%
42	19.063	2882	2886	2893	rVB2	66017	100532	2.35%	0.242%
43	19.157	2898	2902	2904	rBV2	71478	86981	2.03%	0.209%
44	19.269	2914	2921	2924	rBV2	1423256	2042711	47.78%	4.919%
45	19.298	2924	2926	2930	rVB	386294	350288	8.19%	0.843%
46	19.398	2939	2943	2947	rVB3	46492	55213	1.29%	0.133%
47	19.557	2968	2970	2975	rVB	92480	95981	2.25%	0.231%
48	19.769	3001	3006	3009	rBV	91283	116875	2.73%	0.281%
49	19.810	3010	3013	3017	rVB	56441	59779	1.40%	0.144%
50	19.927	3029	3033	3034	rBV3	34492	43318	1.01%	0.104%
51	19.951	3034	3037	3043	rVB2	101873	122220	2.86%	0.294%
52	20.327	3098	3101	3106	rVB2	87956	102068	2.39%	0.246%
53	20.551	3134	3139	3143	rBV	338905	572944	13.40%	1.380%
54	20.674	3157	3160	3164	rVB	60896	70805	1.66%	0.170%
55	20.727	3165	3169	3174	rVB	94433	123264	2.88%	0.297%
56	20.898	3193	3198	3205	rVB	204433	287492	6.72%	0.692%
57	20.968	3205	3210	3216	rVB	277735	372021	8.70%	0.896%
58	21.045	3217	3223	3227	rBV	1064569	1494469	34.96%	3.598%
59	21.168	3240	3244	3250	rVB	85142	130390	3.05%	0.314%
60	21.668	3325	3329	3337	rVB2	69355	123656	2.89%	0.298%
61	22.680	3495	3501	3514	rVB2	124734	303481	7.10%	0.731%
62	23.168	3577	3584	3595	rVB	103214	228572	5.35%	0.550%

Sum of corrected areas: 41530732

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP112719\
Data File : BP001101.D
Acq On : 28 Nov 2019 01:36
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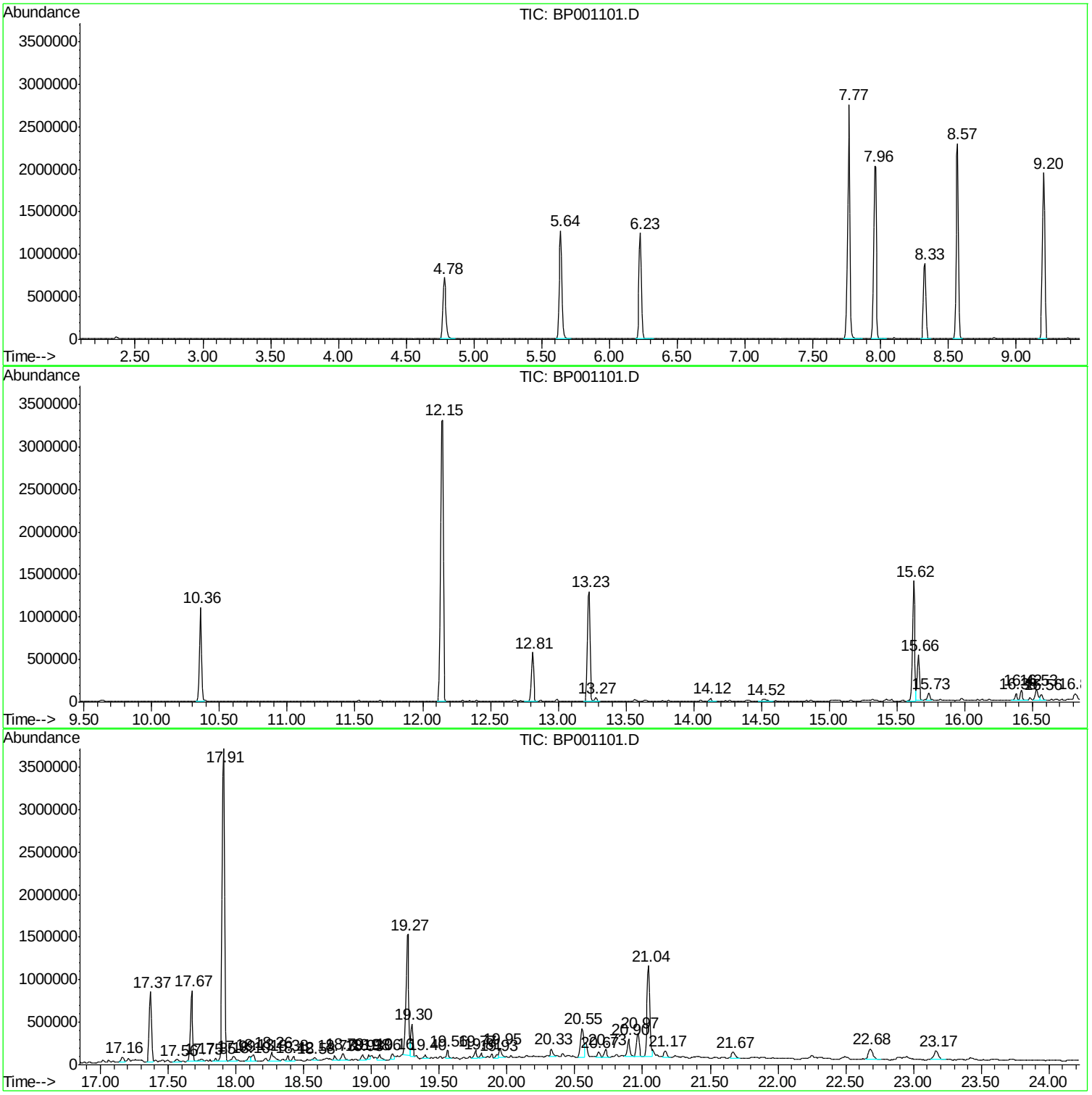
Sample : K5977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WS-112119-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.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\BP112719\
Data File : BP001101.D
Acq On : 28 Nov 2019 01:36
Operator : JU
Sample : K5977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WS-112119-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

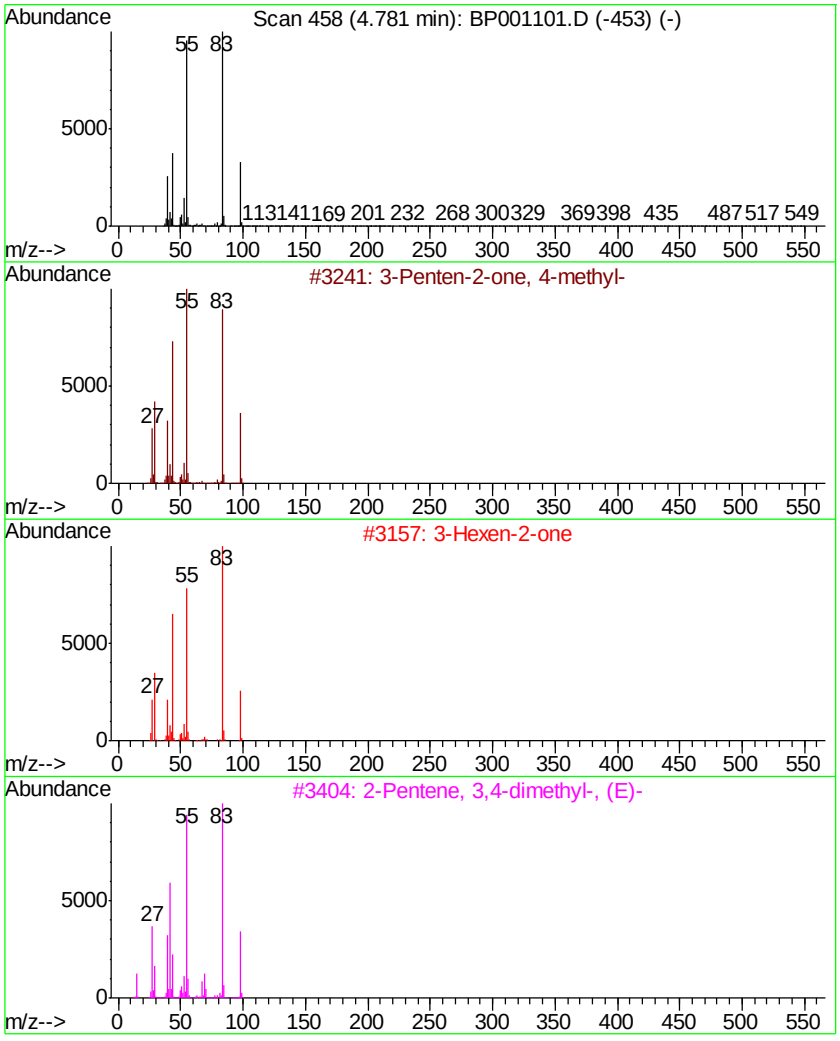
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

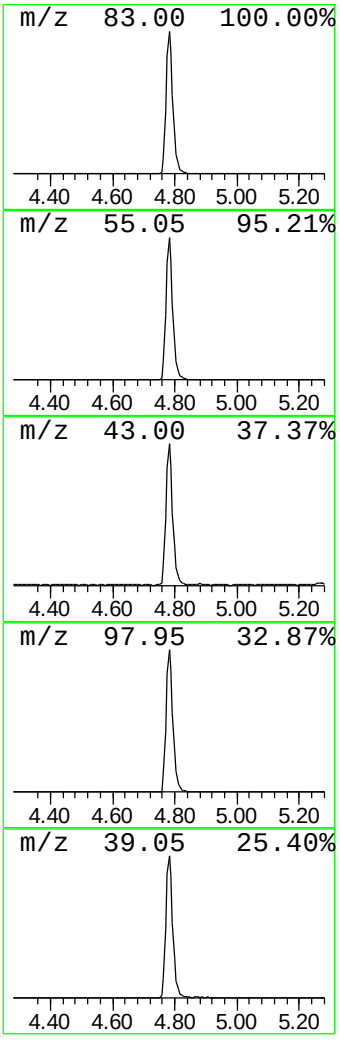
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	21.23 ng	1108110	1,4-Dichlorobenzene-d4	8.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP112719\
Data File : BP001101.D
Acq On : 28 Nov 2019 01:36
Operator : JU
Sample : K5977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WS-112119-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

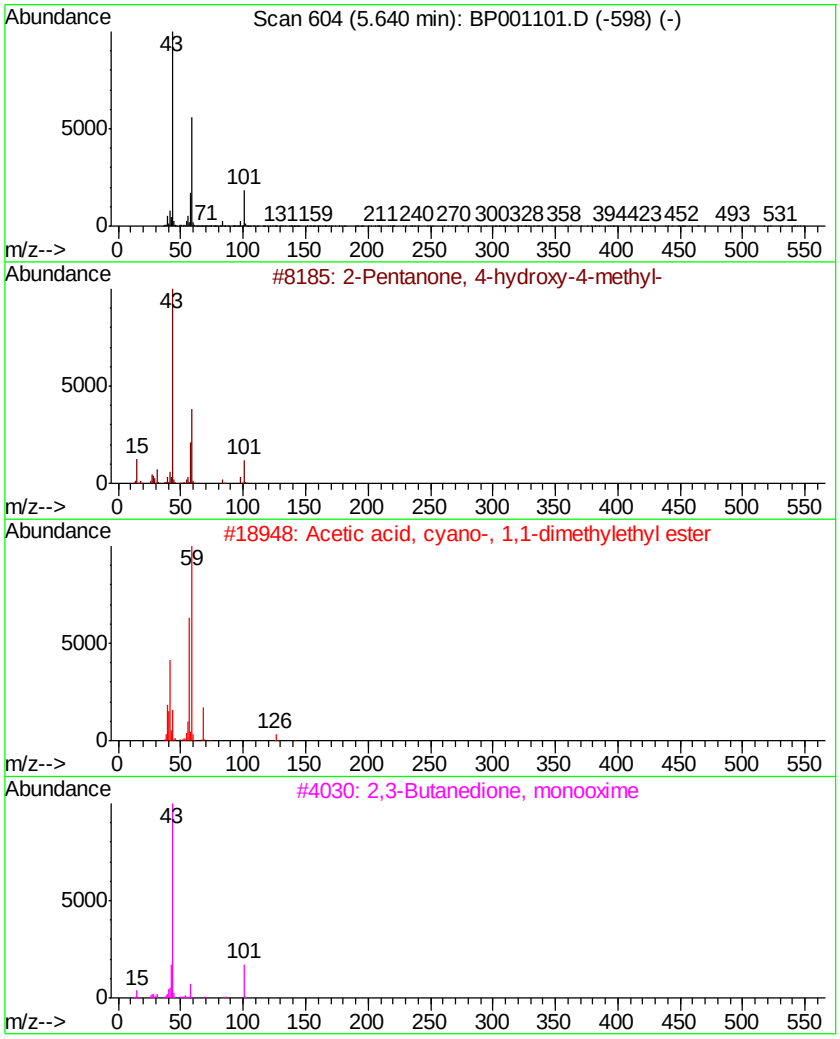
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

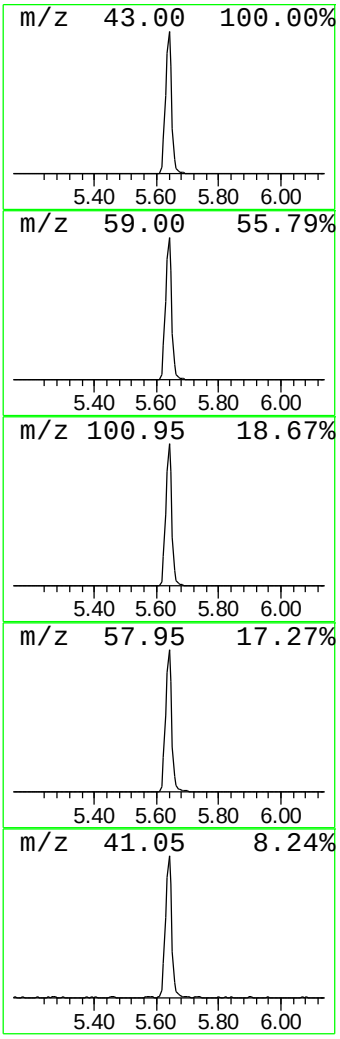
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.64	34.00 ng	1774570	1,4-Dichlorobenzene-d4	8.33

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP112719\
Data File : BP001101.D
Acq On : 28 Nov 2019 01:36
Operator : JU
Sample : K5977-02
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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WS-112119-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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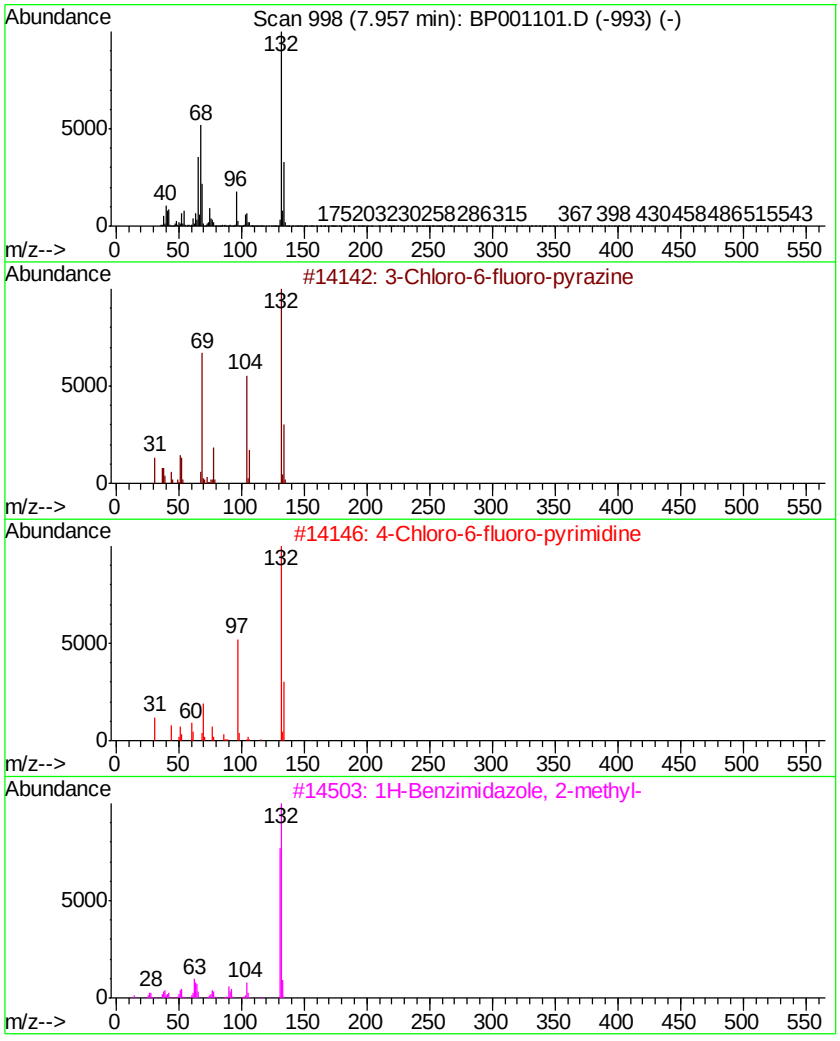
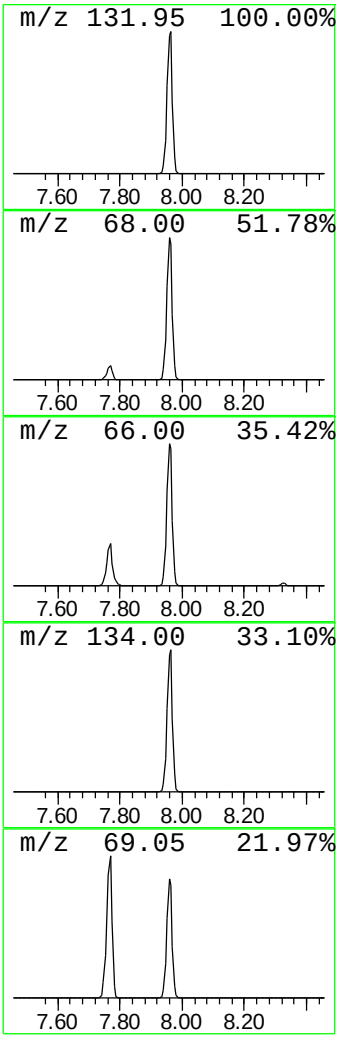
Peak Number 3 unknown7.96 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.96	49.81 ng	2599940	1,4-Dichlorobenzene-d4	8.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Sample : K5977-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WS-112119-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
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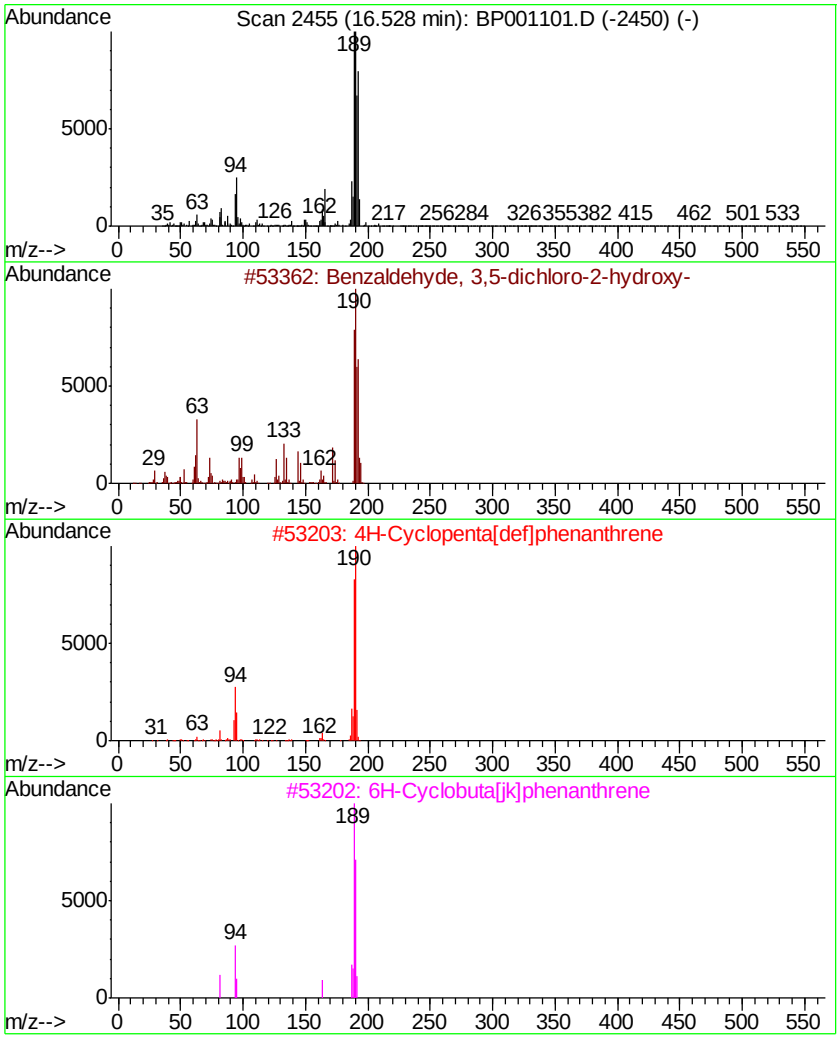
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

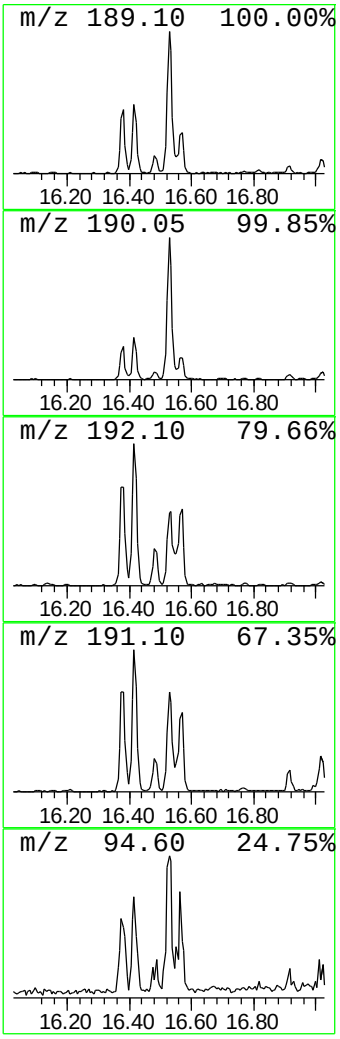
****

Peak Number 5 Benzaldehyde, 3,5-dichloro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.10 ng	171683	Phenanthrene-d10	15.62

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	58
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38





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ALS Vial : 18 Sample Multiplier: 1

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ClientSampleId : WS-112119-0-2-COMP-B1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

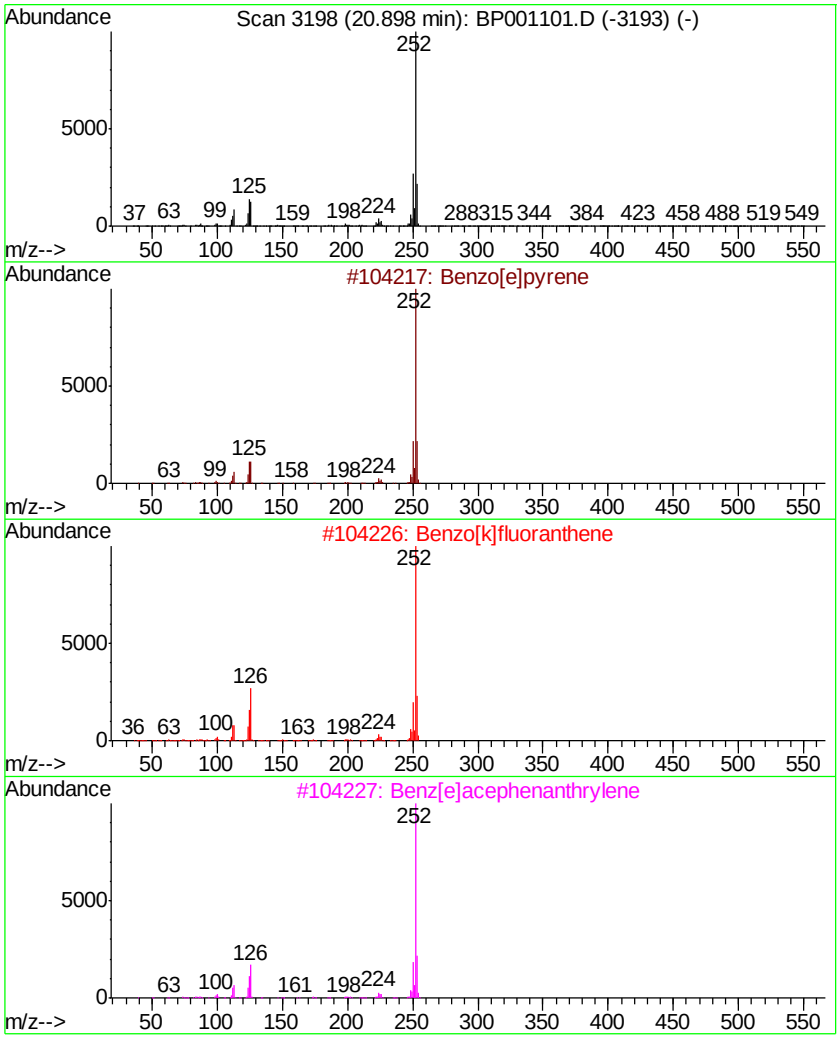
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

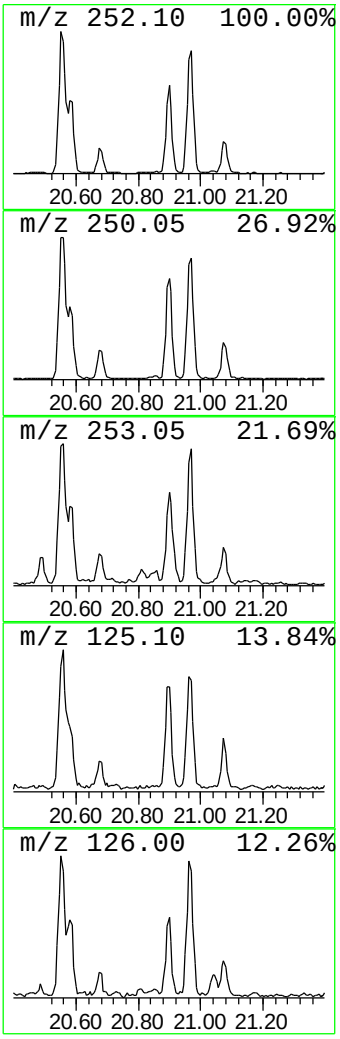
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.90	3.85 ng	287492	Perylene-d12	21.05

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	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_P
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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
3-Penten-2-one, 4...	4.78	21.2	ng	1108110	1	8.33	1043900	20.0
2-Pentanone, 4-hy...	5.64	34.0	ng	1774570	1	8.33	1043900	20.0
unknown7.96	7.96	49.8	ng	2599940	1	8.33	1043900	20.0
Benzaldehyde, 3,5...	16.53	2.1	ng	171683	4	15.62	1637390	20.0
Benzo[e]pyrene	20.90	3.9	ng	287492	6	21.05	1494470	20.0