LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033121\
Data File : BP005124.D
Acq On : 31 Mar 2021 13:55
Operator : CG/JU
Sample : M1823-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MK-3-29-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\8270E-BP032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005124.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.863	292	302	310	rVB	18556	31847	3.21%	0.340%
2	5.310	372	378	385	rBV	231501	333612	33.59%	3.557%
3	5.740	444	451	458	rVB9	6188	13654	1.37%	0.146%
4	6.893	637	647	660	rVB	225801	362798	36.52%	3.868%
5	7.340	718	723	725	rBV	9090	12936	1.30%	0.138%
6	7.716	777	787	794	rBV	158909	250219	25.19%	2.668%
7	8.252	869	878	883	rBV7	5762	15152	1.53%	0.162%
8	8.875	977	984	990	rBV	142212	225603	22.71%	2.405%
9	8.940	990	995	1005	rVB2	19921	31239	3.14%	0.333%
10	10.504	1252	1261	1267	rBV	194712	342198	34.45%	3.648%
11	10.551	1267	1269	1276	rVB2	8005	12611	1.27%	0.134%
12	11.940	1499	1505	1513	rVB3	6498	11133	1.12%	0.119%
13	12.175	1534	1545	1551	rVB3	8259	16908	1.70%	0.180%
14	12.392	1576	1582	1593	rBV5	5879	11642	1.17%	0.124%
15	12.987	1676	1683	1692	rVB	349829	521352	52.49%	5.558%
16	13.192	1713	1718	1724	rVB7	9814	14785	1.49%	0.158%
17	13.687	1797	1802	1805	rBV4	8180	12754	1.28%	0.136%
18	13.828	1822	1826	1829	rBV2	12671	19755	1.99%	0.211%
19	14.092	1866	1871	1876	rBV	16097	24340	2.45%	0.259%
20	14.216	1885	1892	1898	rBV9	5112	13868	1.40%	0.148%
21	14.275	1898	1902	1908	rVV3	9399	13336	1.34%	0.142%
22	14.369	1911	1918	1924	rVV	291916	429785	43.27%	4.582%
23	14.434	1924	1929	1938	rVB	24380	40121	4.04%	0.428%
24	14.769	1982	1986	1994	rVB	18565	32312	3.25%	0.344%
25	14.845	1994	1999	2004	rBV6	6360	9956	1.00%	0.106%
26	15.233	2062	2065	2070	rVB5	7491	11828	1.19%	0.126%
27	15.422	2092	2097	2101	rBV	34559	49903	5.02%	0.532%
28	15.633	2130	2133	2139	rBV8	8444	12577	1.27%	0.134%
29	15.722	2145	2148	2154	rVB4	9225	16415	1.65%	0.175%
30	15.869	2166	2173	2180	rVB	281669	415319	41.81%	4.428%
31	16.098	2208	2212	2221	rBV7	14316	35183	3.54%	0.375%
32	16.433	2263	2269	2273	rBV4	9387	16249	1.64%	0.173%
33	16.898	2345	2348	2352	rVV6	8175	10045	1.01%	0.107%
34	16.951	2352	2357	2364	rVB	18464	34387	3.46%	0.367%
35	17.128	2382	2387	2391	rBV	331321	477542	48.08%	5.091%
36	17.169	2391	2394	2401	rVV	205420	284158	28.61%	3.029%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033121\
Data File : BP005124.D
Acq On : 31 Mar 2021 13:55
Operator : CG/JU
Sample : M1823-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MK-3-29-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\8270E-BP032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.263	2405	2410	2415	rVB	85457	120153	12.10%	1.281%
38	17.539	2453	2457	2462	rBV	11118	22249	2.24%	0.237%
39	17.639	2470	2474	2479	rBV8	10827	23883	2.40%	0.255%
40	17.810	2500	2503	2507	rVB2	14606	20269	2.04%	0.216%
41	17.857	2507	2511	2513	rBV5	7469	12531	1.26%	0.134%
42	18.004	2532	2536	2537	rBV	33097	38104	3.84%	0.406%
43	18.027	2537	2540	2550	rVB4	117982	206736	20.81%	2.204%
44	18.127	2554	2557	2562	rVB2	27447	37469	3.77%	0.399%
45	18.192	2563	2568	2572	rBV2	70071	117684	11.85%	1.255%
46	18.310	2583	2588	2592	rBV4	20162	37533	3.78%	0.400%
47	18.498	2615	2620	2625	rBV2	41062	89945	9.05%	0.959%
48	18.951	2694	2697	2700	rVB4	33359	40450	4.07%	0.431%
49	19.151	2726	2731	2738	rBV	490717	657567	66.20%	7.010%
50	19.269	2748	2751	2754	rBV	45879	54069	5.44%	0.576%
51	19.504	2782	2791	2799	rBV	414570	703839	70.86%	7.503%
52	19.704	2820	2825	2829	rVB	604153	716629	72.14%	7.640%
53	19.986	2870	2873	2879	rVB	90345	122618	12.34%	1.307%
54	20.086	2887	2890	2893	rVB	94428	109360	11.01%	1.166%
55	21.221	3077	3083	3087	rBV2	529793	993322	100.00%	10.590%
56	21.263	3087	3090	3095	rVB	218004	292696	29.47%	3.120%
57	22.821	3351	3355	3360	rBV	157651	309251	31.13%	3.297%
58	23.515	3469	3473	3479	rVB	286216	486268	48.95%	5.184%

Sum of corrected areas: 9380147

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Acq On : 31 Mar 2021 13:55
Operator : CG/JU
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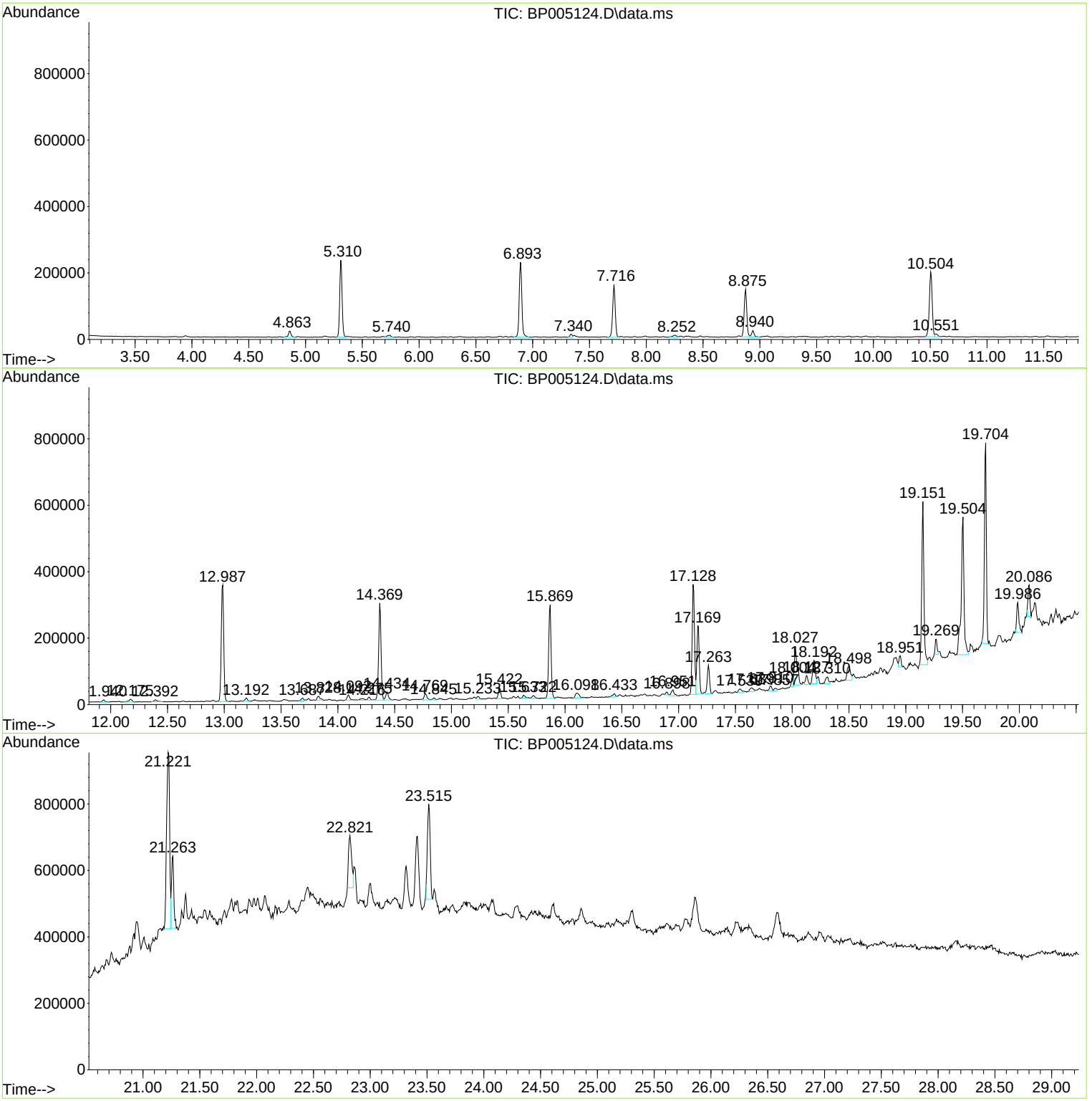
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MK-3-29-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.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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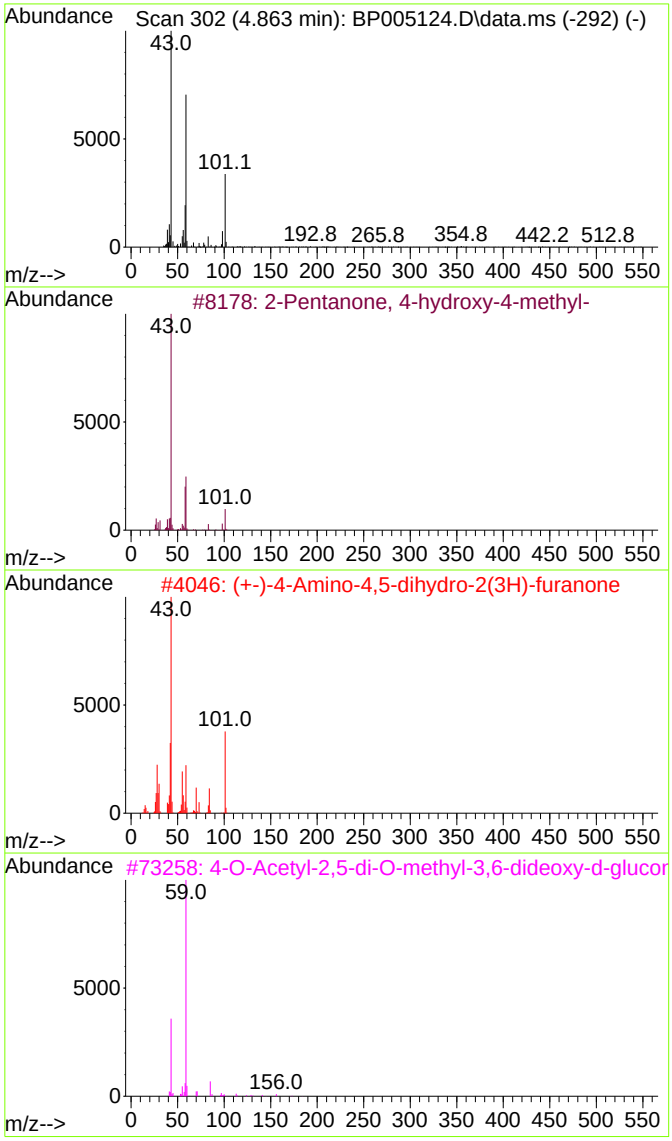
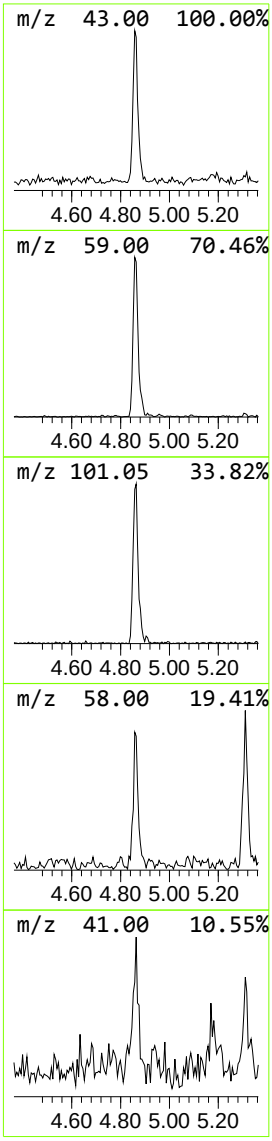
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.863	2.55 ng	31847	1,4-Dichlorobenzene-d4	7.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	4-O-Acetyl-2,5-di-O-methyl-3,6-d...	215	C10H17NO4	1000101-80-3	37
4	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	25
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	25





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Operator : CG/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MK-3-29-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

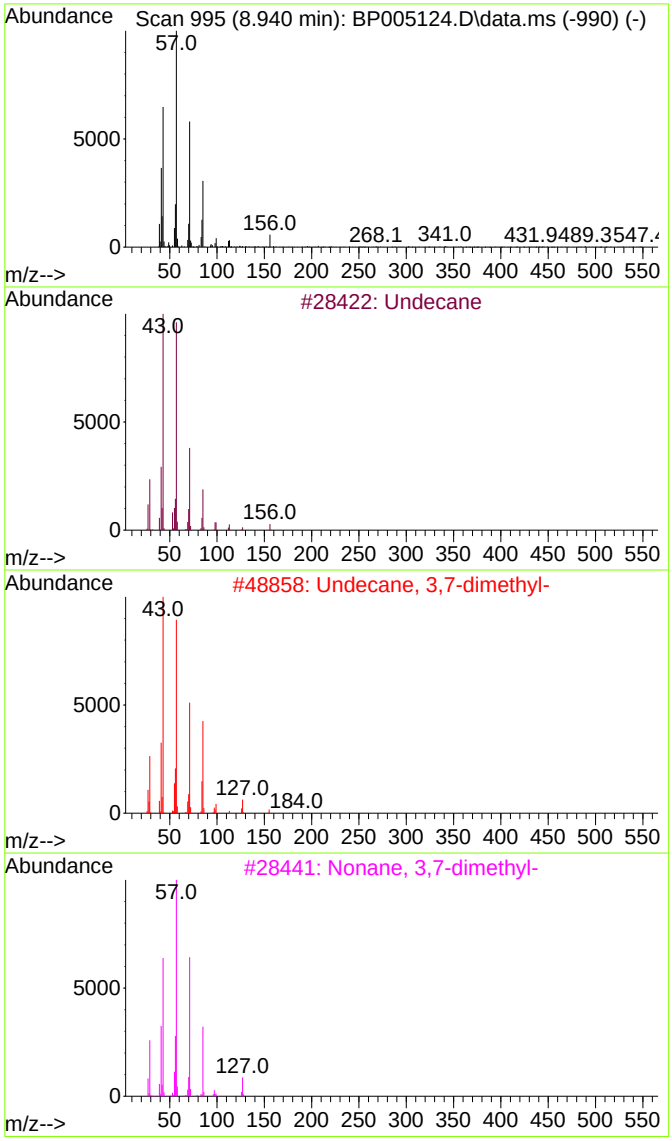
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

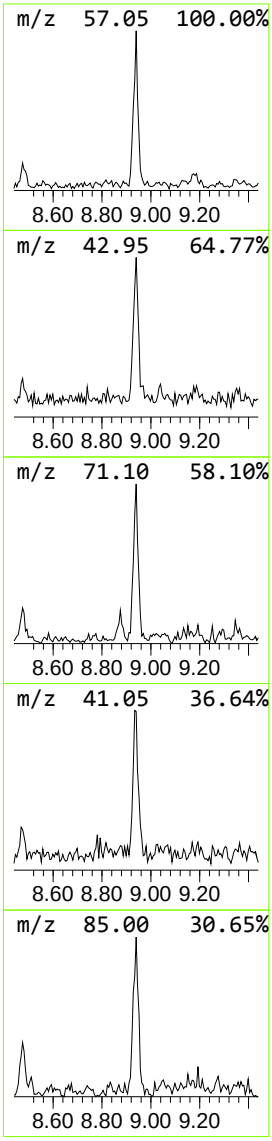
****

Peak Number 2 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.940	2.50 ng	31239	1,4-Dichlorobenzene-d4	7.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	90
2	Undecane, 3,7-dimethyl-	184	C13H28	017301-29-0	64
3	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	64
4	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
5	Decane, 2,3,7-trimethyl-	184	C13H28	062238-13-5	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033121\
Data File : BP005124.D
Acq On : 31 Mar 2021 13:55
Operator : CG/JU
Sample : M1823-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MK-3-29-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

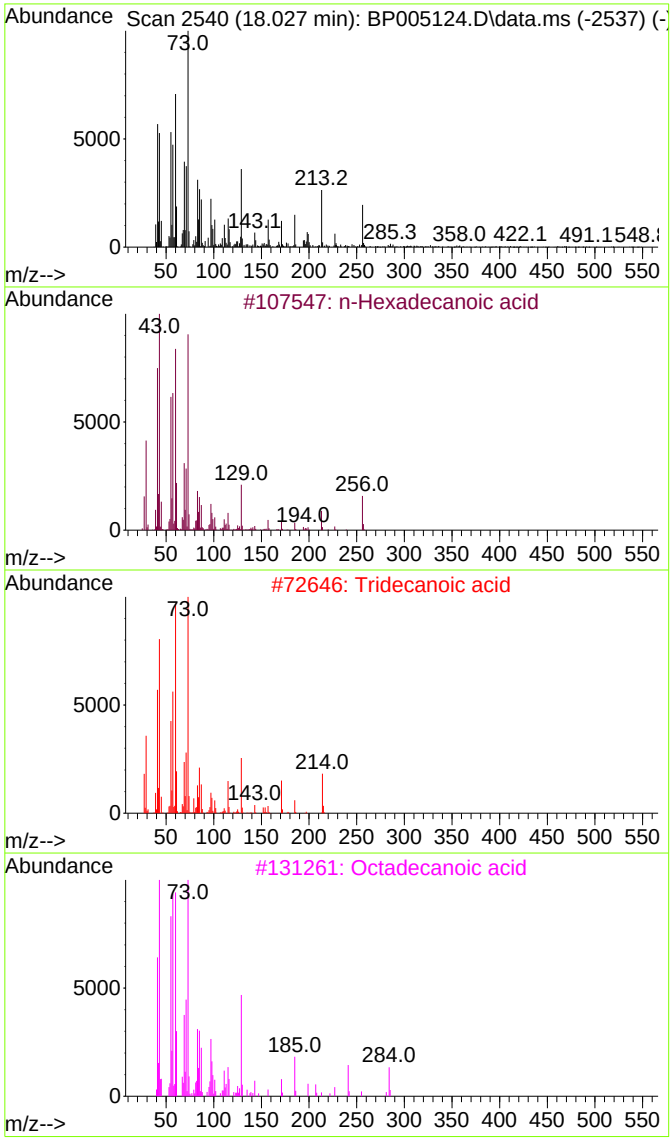
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

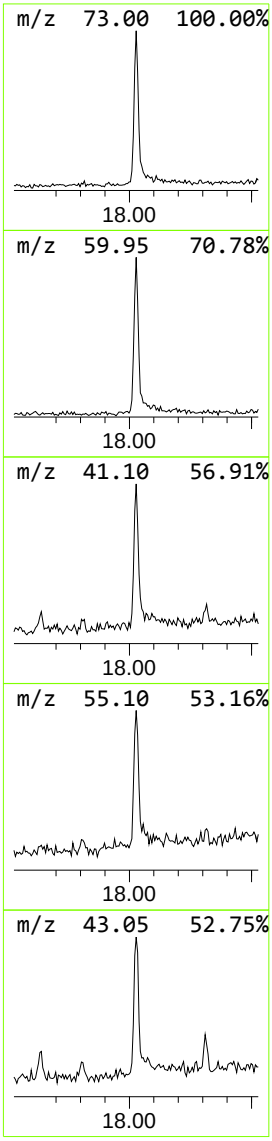
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.028	8.66 ng	206736	Phenanthrene-d10	17.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	62
3	Octadecanoic acid	284	C18H36O2	000057-11-4	50
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033121\
Data File : BP005124.D
Acq On : 31 Mar 2021 13:55
Operator : CG/JU
Sample : M1823-01 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MK-3-29-B1

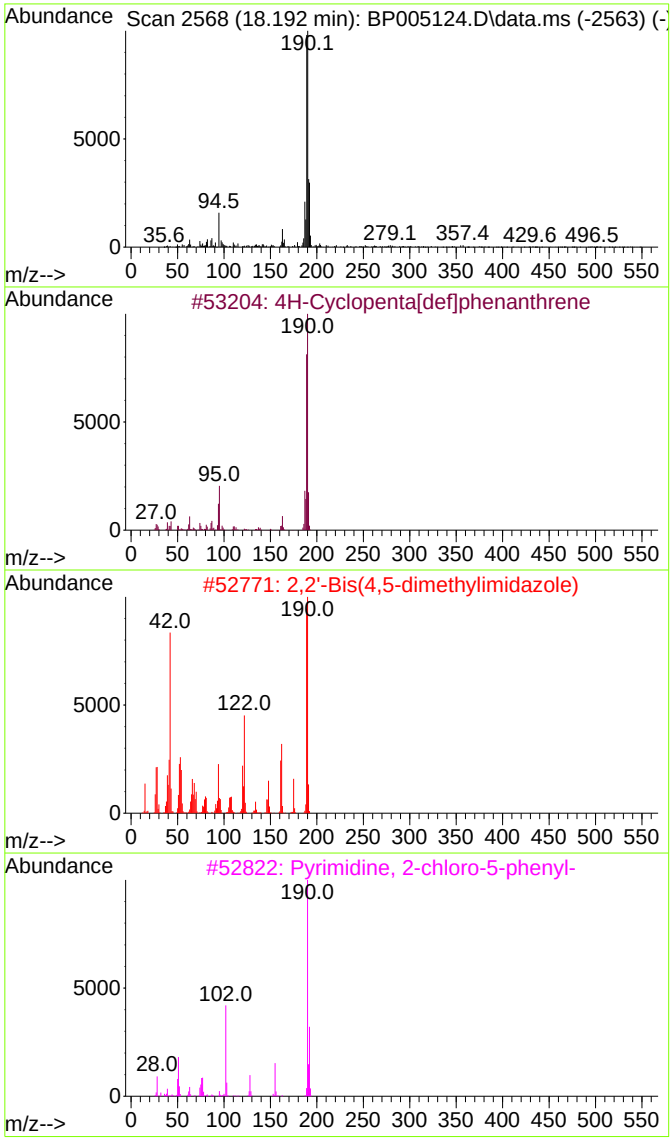
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

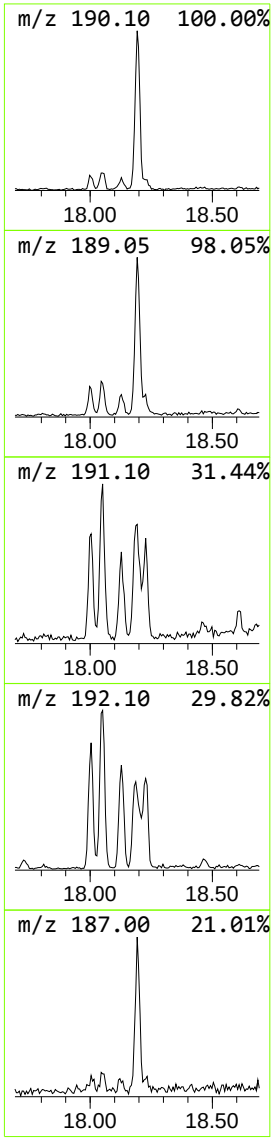
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	4.93 ng	117684	Phenanthrene-d10	17.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
3	Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	35
4	2,6-Dichlorobenzaldoxime	189	C7H5Cl2NO	025185-95-9	30
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27





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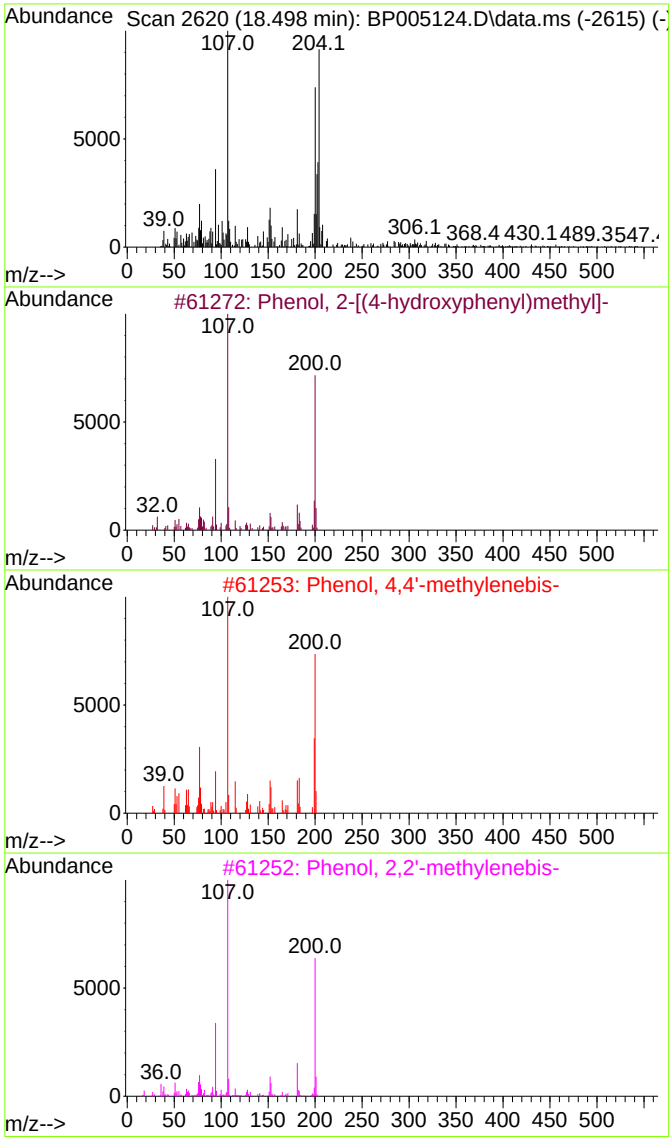
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

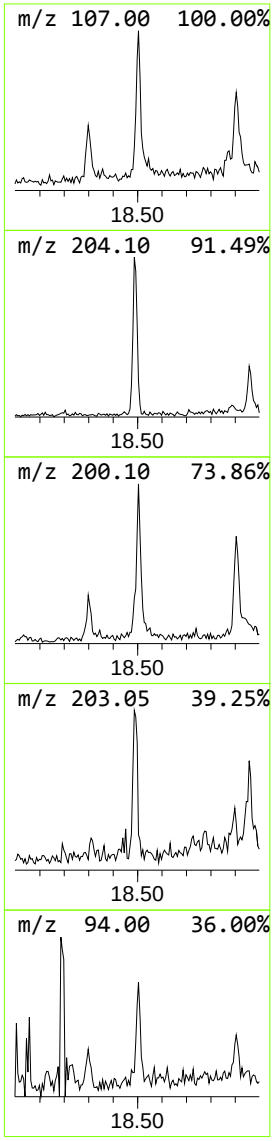
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenol, 2-[(4-hydroxyphenyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.498	3.77 ng	89945	Phenanthrene-d10	17.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	55
2	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	50
3	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	45
4	3-Isopropylidene-tricyclo[4.3.1....	204	C14H20O	1000194-65-4	38
5	Propenone, 3-(5-trifluoromethyl-...	309	C15H10F3NOS	284496-12-4	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

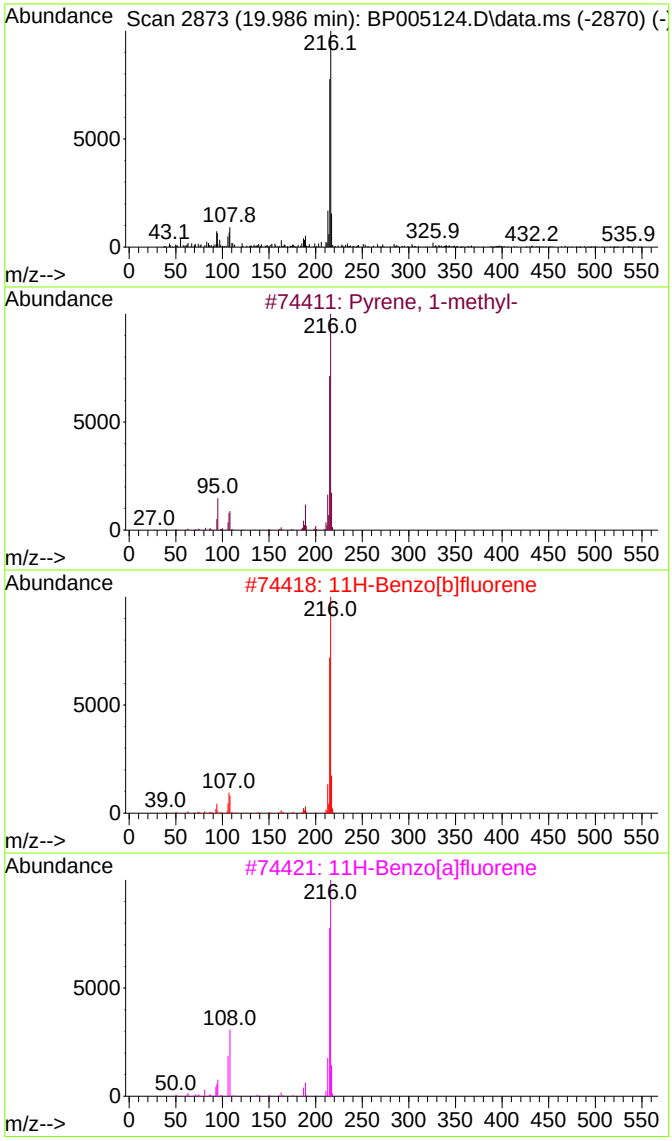
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

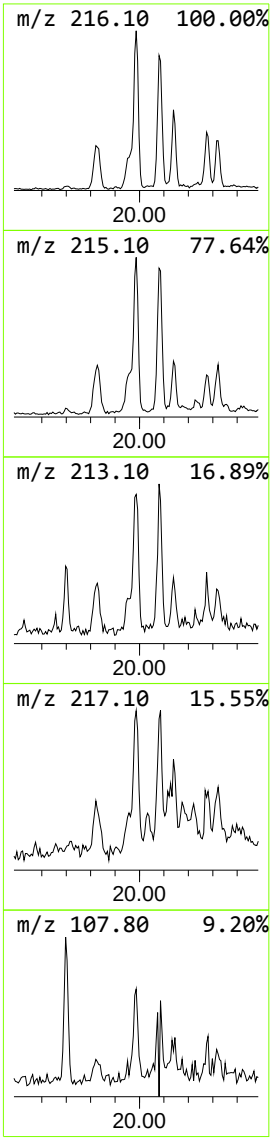
****

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.986	2.47 ng	122618	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	64





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MK-3-29-B1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

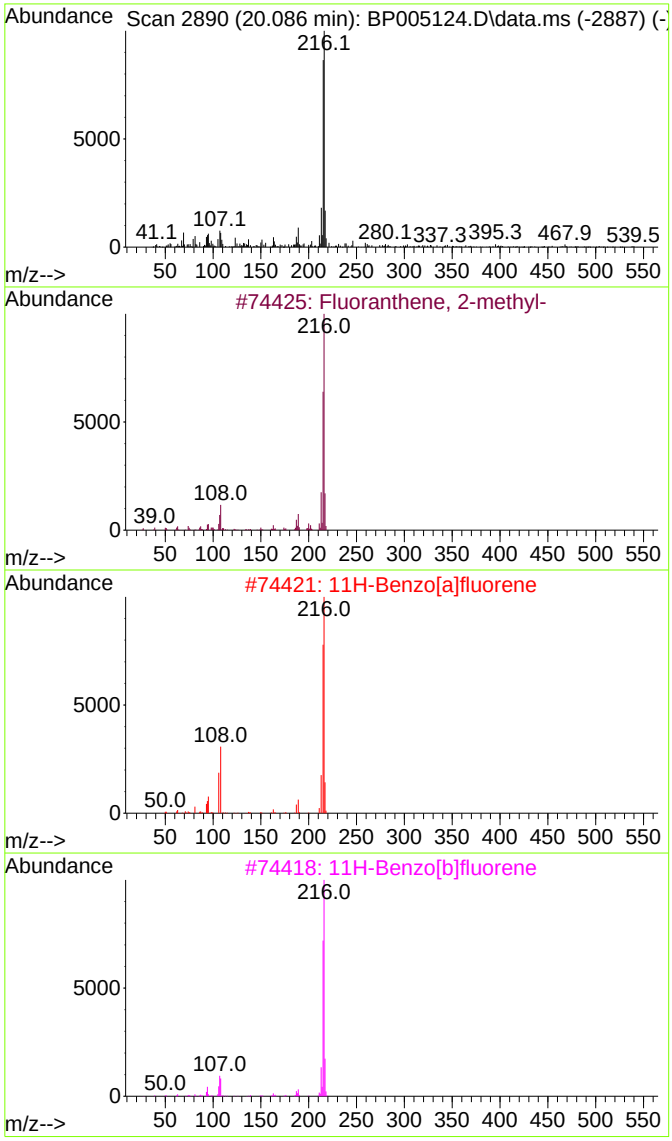
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

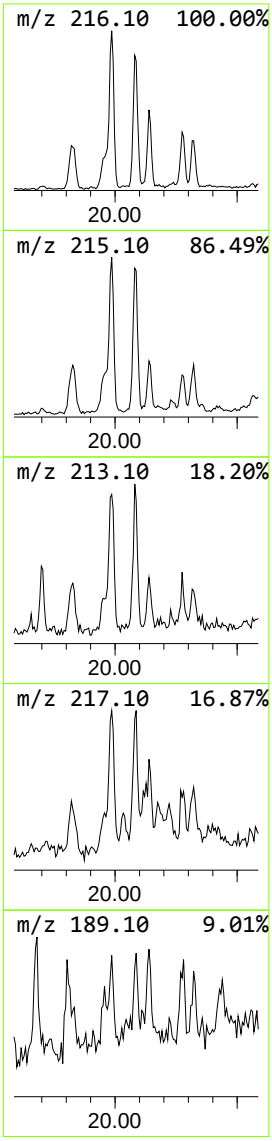
****

Peak Number 8 Fluoranthene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.086	2.20 ng	109360	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
5	Benzoic acid, 3-(3,5-dimethyl-1-...	216	C12H12N2O2	312531-88-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033121\
Data File : BP005124.D
Acq On : 31 Mar 2021 13:55
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.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
2-Pentanone, 4-...	4.863	2.5	ng	31847	1	7.716	250219	20.0
Undecane	8.940	2.5	ng	31239	1	7.716	250219	20.0
n-Hexadecanoic ...	18.028	8.7	ng	206736	4	17.128	477542	20.0
4H-Cyclopenta[d...	18.192	4.9	ng	117684	4	17.128	477542	20.0
Phenol, 2-[(4-h...	18.498	3.8	ng	89945	4	17.128	477542	20.0
Pyrene, 1-methyl-	19.986	2.5	ng	122618	5	21.227	993322	20.0
Fluoranthene, 2...	20.086	2.2	ng	109360	5	21.227	993322	20.0