LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004127.D
Acq On : 02 Dec 2020 13:53
Operator : CG/JU
Sample : L4911-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SK-12-1-SPE

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-BP110320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004127.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.210	337	344	352	rBV	43026	63127	1.73%	0.230%
2	5.734	426	433	445	rBV	1721608	2583728	70.70%	9.427%
3	6.134	496	501	507	rBV	28717	44016	1.20%	0.161%
4	7.381	706	713	729	rBV	1621412	2648023	72.46%	9.662%
5	8.193	844	851	859	rBV	472091	736963	20.17%	2.689%
6	9.357	1042	1049	1058	rVB	1023289	1656889	45.34%	6.046%
7	11.022	1324	1332	1338	rBV	552862	935019	25.59%	3.412%
8	13.445	1737	1744	1752	rVB	2096846	3056909	83.65%	11.154%
9	14.251	1876	1881	1885	rBV	65007	83852	2.29%	0.306%
10	14.628	1940	1945	1955	rVB3	25604	57177	1.56%	0.209%
11	14.822	1972	1978	1985	rVB	729098	1071287	29.32%	3.909%
12	15.363	2063	2070	2077	rBV2	27772	50780	1.39%	0.185%
13	15.939	2163	2168	2175	rBV	20244	47327	1.30%	0.173%
14	16.310	2224	2231	2238	rBV	1535457	2136248	58.46%	7.795%
15	16.575	2272	2276	2282	rVB3	25104	43562	1.19%	0.159%
16	16.928	2331	2336	2347	rBV4	56086	108187	2.96%	0.395%
17	17.557	2437	2443	2448	rBV	802805	1187953	32.51%	4.335%
18	17.604	2448	2451	2458	rVB	130769	170707	4.67%	0.623%
19	18.410	2584	2588	2592	rBV	89469	121541	3.33%	0.443%
20	18.463	2592	2597	2603	rVB2	77910	111901	3.06%	0.408%
21	18.592	2615	2619	2623	rBV2	61873	114951	3.15%	0.419%
22	18.633	2624	2626	2629	rVV	60607	75586	2.07%	0.276%
23	18.674	2629	2633	2636	rVV	113285	164739	4.51%	0.601%
24	18.716	2636	2640	2650	rVB	90177	161678	4.42%	0.590%
25	18.922	2672	2675	2685	rVB3	31637	55886	1.53%	0.204%
26	19.122	2705	2709	2713	rBV2	28109	37658	1.03%	0.137%
27	19.292	2734	2738	2742	rBV	52954	78288	2.14%	0.286%
28	19.427	2757	2761	2766	rBV4	33278	54463	1.49%	0.199%
29	19.545	2776	2781	2786	rVB	179446	233563	6.39%	0.852%
30	19.863	2831	2835	2836	rBV2	40222	45358	1.24%	0.165%
31	19.892	2836	2840	2848	rVB	278783	389882	10.67%	1.423%
32	20.069	2864	2870	2875	rBV	3015051	3654350	100.00%	13.334%
33	20.521	2944	2947	2950	rVB	49919	53479	1.46%	0.195%
34	20.657	2967	2970	2973	rBV	55708	66171	1.81%	0.241%
35	20.704	2975	2978	2981	rVB	47922	50724	1.39%	0.185%
36	20.774	2984	2990	2991	rBV2	79668	152307	4.17%	0.556%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004127.D
Acq On : 02 Dec 2020 13:53
Operator : CG/JU
Sample : L4911-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SK-12-1-SPE

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-BP110320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.086	3041	3043	3049	rVB	53978	66247	1.81%	0.242%
38	21.257	3068	3072	3081	rVB3	394392	604502	16.54%	2.206%
39	21.327	3081	3084	3088	rBV	134165	154297	4.22%	0.563%
40	21.598	3124	3130	3134	rBV2	1025230	1544438	42.26%	5.635%
41	21.639	3134	3137	3144	rVB	156226	213666	5.85%	0.780%
42	21.927	3178	3186	3200	rVB7	181556	643919	17.62%	2.349%
43	22.074	3206	3211	3222	rBV4	105370	328924	9.00%	1.200%
44	23.298	3415	3419	3425	rBV2	97387	195430	5.35%	0.713%
45	24.039	3538	3545	3552	rBV	698768	1351133	36.97%	4.930%

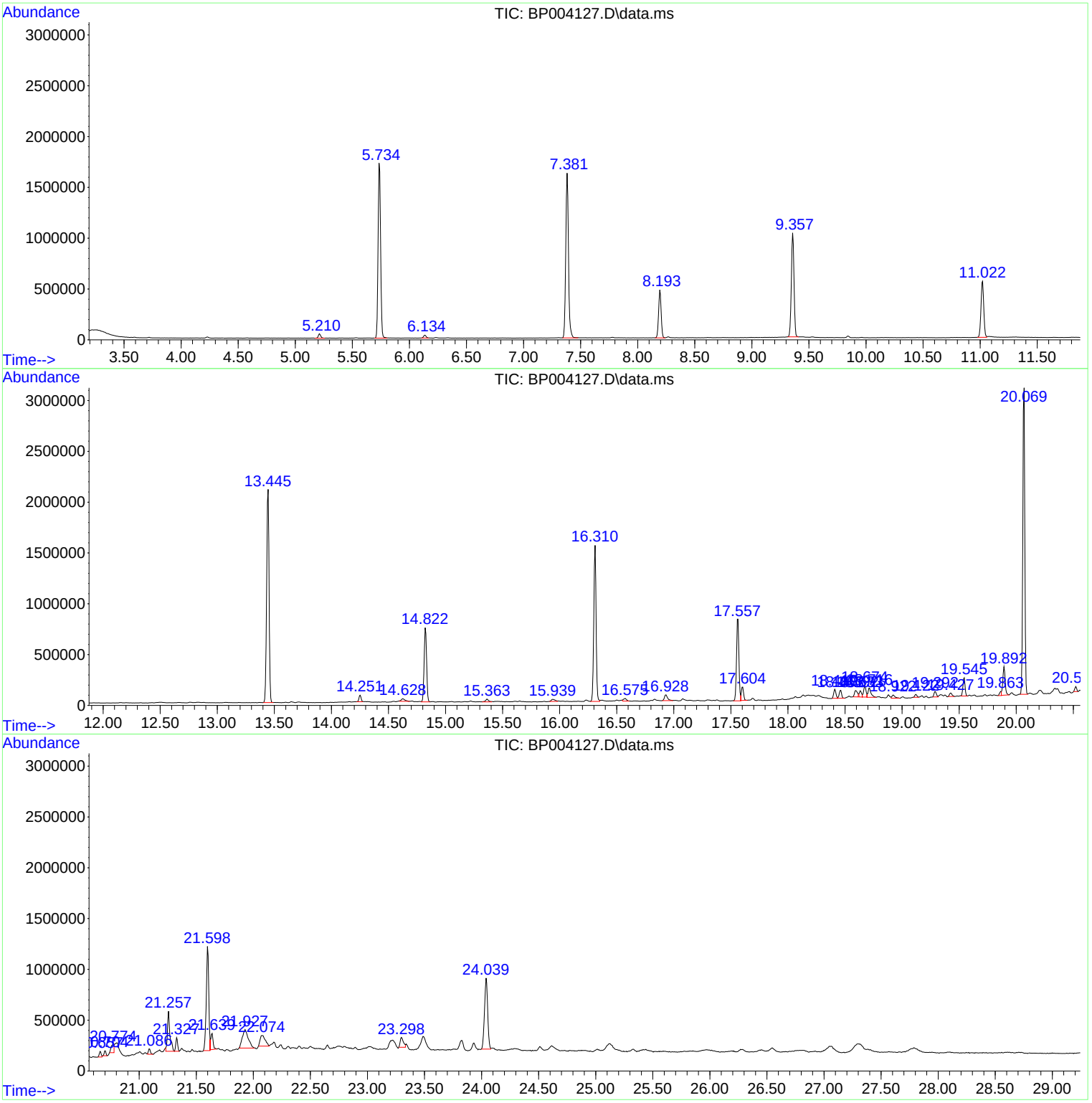
Sum of corrected areas: 27406835

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004127.D
Acq On : 02 Dec 2020 13:53
Operator : CG/JU
Sample : L4911-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SK-12-1-SPE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-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\BP120220\
Data File : BP004127.D
Acq On : 02 Dec 2020 13:53
Operator : CG/JU
Sample : L4911-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SK-12-1-SPE

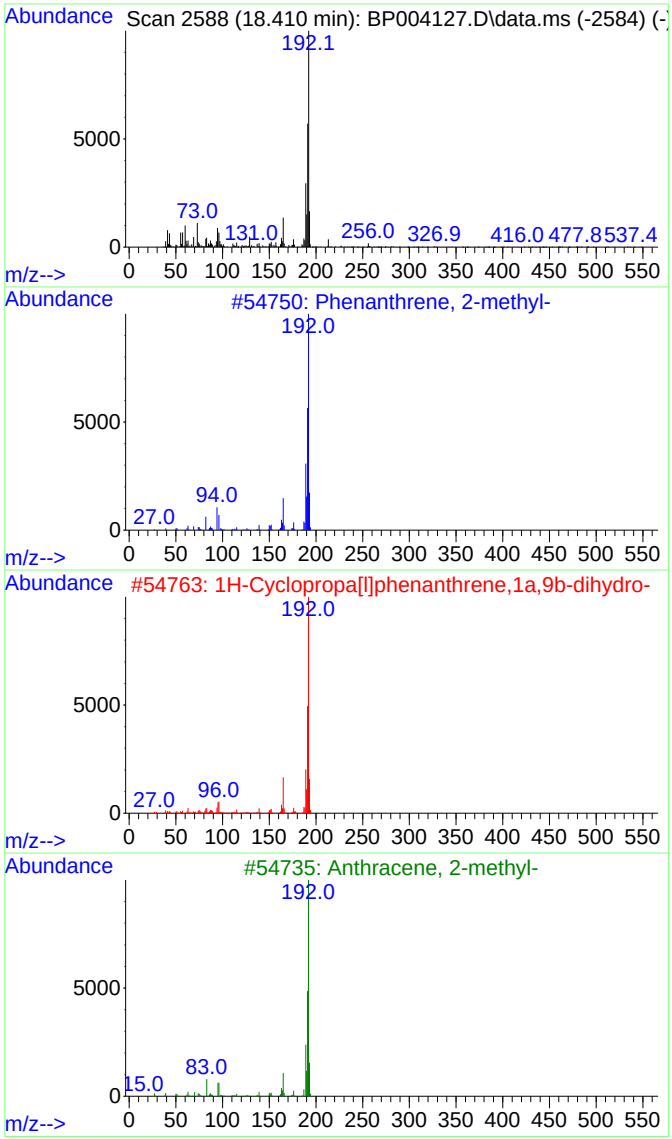
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

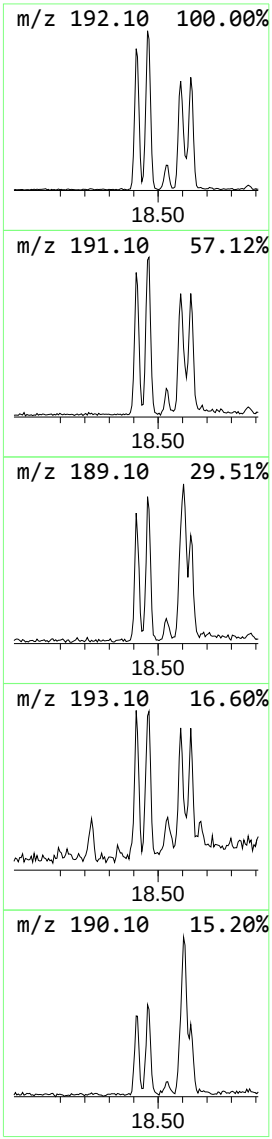
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.410	2.05 ng	121541	Phenanthrene-d10	17.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	97
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	97
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	96
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004127.D
Acq On : 02 Dec 2020 13:53
Operator : CG/JU
Sample : L4911-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SK-12-1-SPE

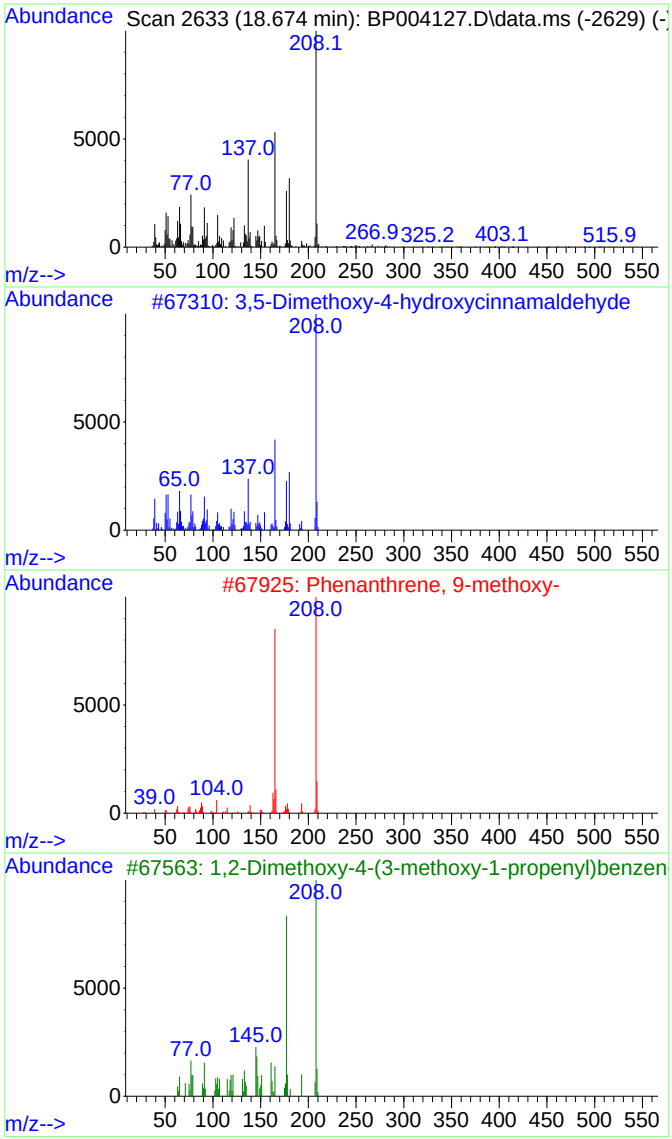
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

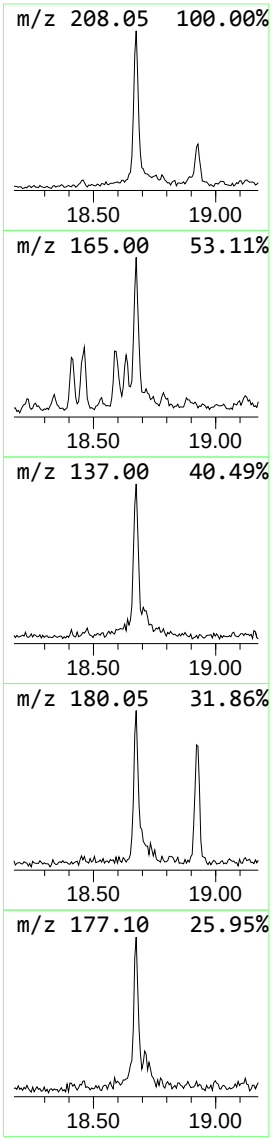
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.674	2.77 ng	164739	Phenanthrene-d10	17.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	89
2	Phenanthrene, 9-methoxy-	208	C15H12O	005085-74-5	45
3	1,2-Dimethoxy-4-(3-methoxy-1-pro...	208	C12H16O3	1000313-35-0	43
4	3,4-Dimethoxycinnamic acid	208	C11H12O4	002316-26-9	38
5	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004127.D
Acq On : 02 Dec 2020 13:53
Operator : CG/JU
Sample : L4911-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SK-12-1-SPE

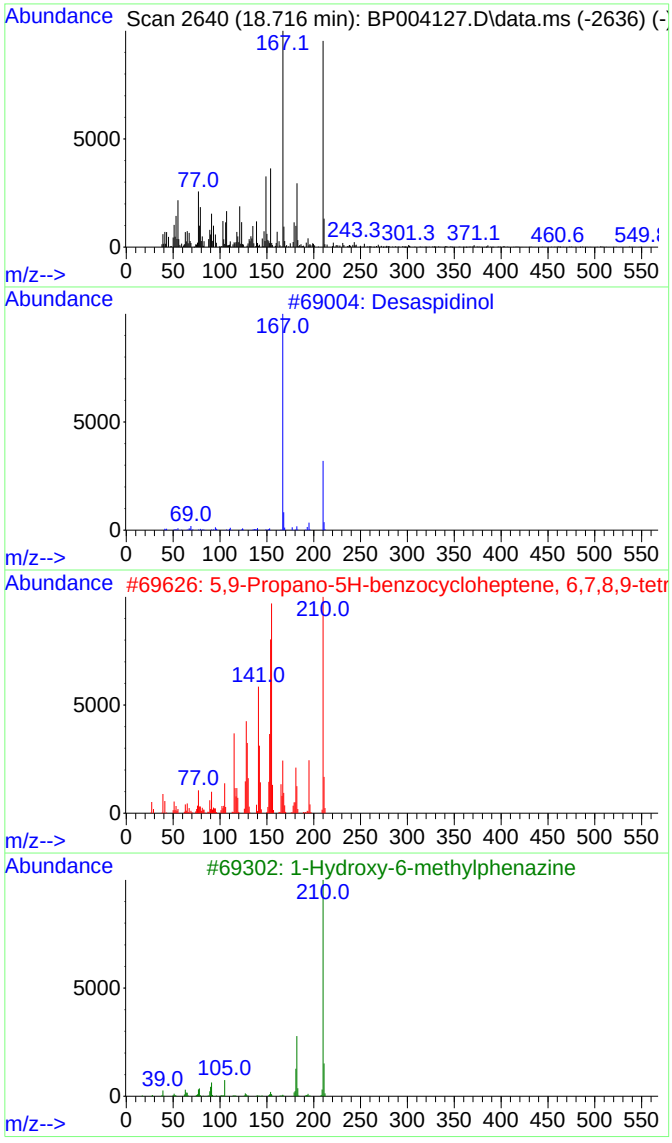
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

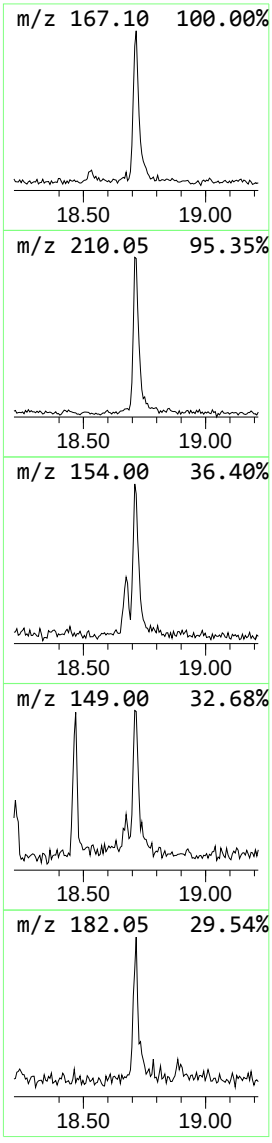
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Desaspidinol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.716	2.72 ng	161678	Phenanthrene-d10	17.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Desaspidinol	210	C11H14O4	000437-72-9	53
2	5,9-Propano-5H-benzocycloheptene...	210	C16H18	073947-11-2	43
3	1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	41
4	9-Methyl-1-phenazinol	210	C13H10N2O	013860-43-0	38
5	1,1'-Biphenyl, 3,3',4,4'-tetrame...	210	C16H18	004920-95-0	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004127.D
Acq On : 02 Dec 2020 13:53
Operator : CG/JU
Sample : L4911-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SK-12-1-SPE

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

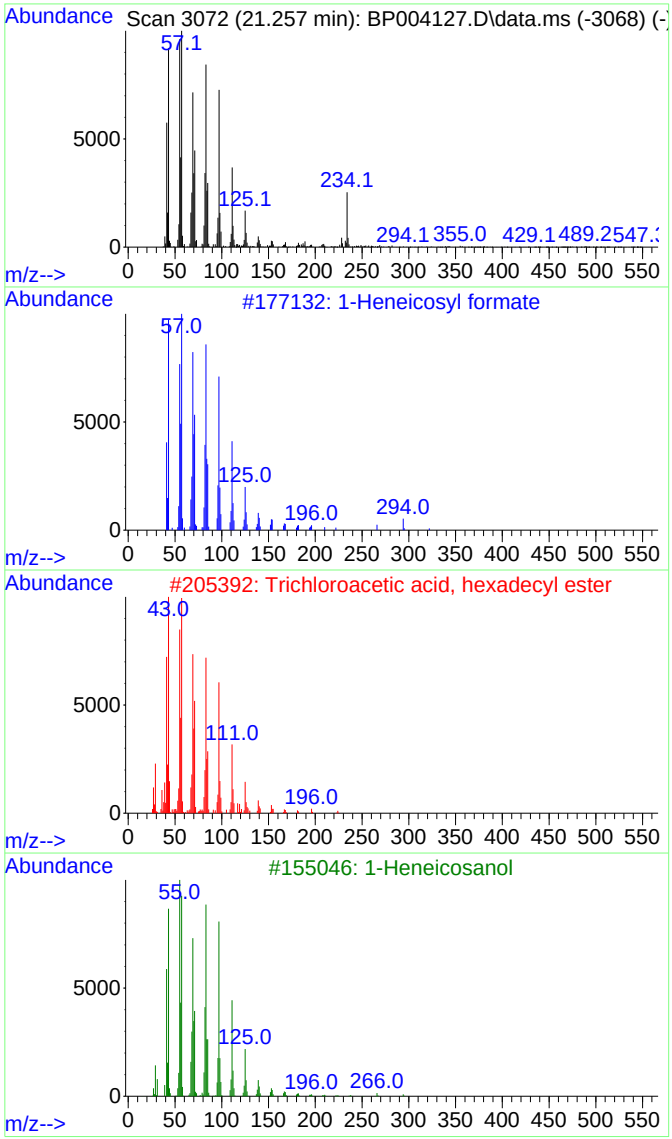
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

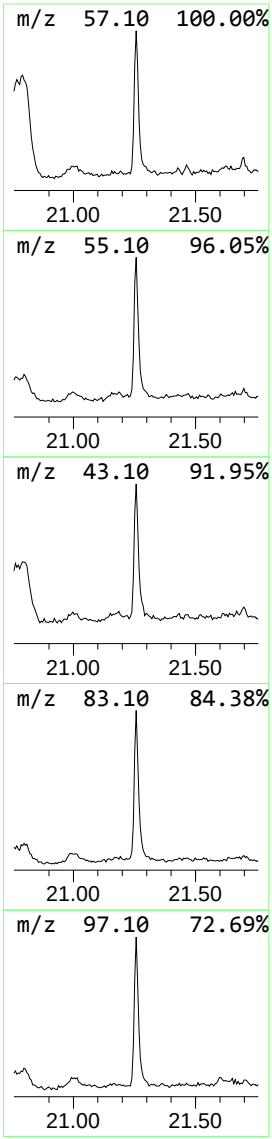
****

Peak Number 4 1-Heneicosyl formate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.257	7.83 ng	604502	Chrysene-d12	21.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	98
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	1-Docosene	308	C22H44	001599-67-3	93
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	92





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004127.D
Acq On : 02 Dec 2020 13:53
Operator : CG/JU
Sample : L4911-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SK-12-1-SPE

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

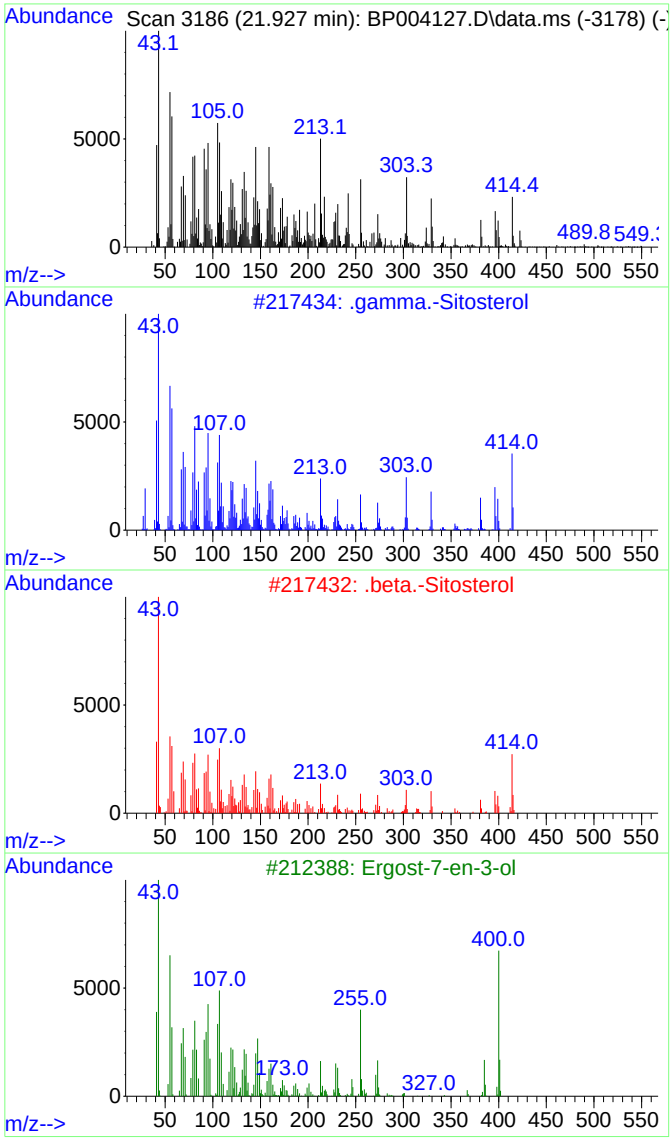
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

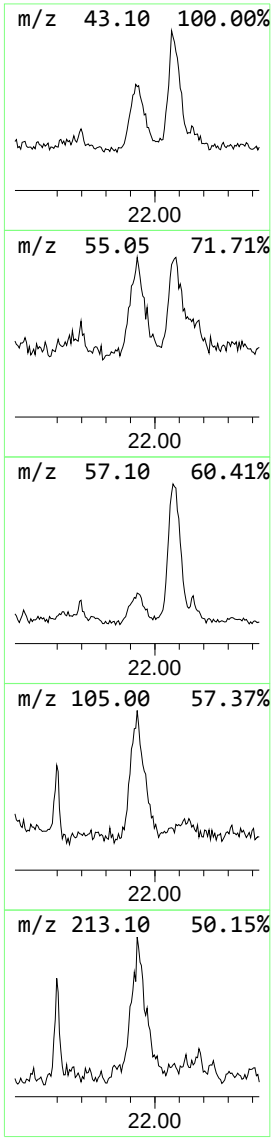
****

Peak Number 5 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.927	8.34 ng	643919	Chrysene-d12	21.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	97
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	92
3	Ergost-7-en-3-ol	400	C28H48O	116179-22-7	53
4	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	43
5	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004127.D
Acq On : 02 Dec 2020 13:53
Operator : CG/JU
Sample : L4911-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SK-12-1-SPE

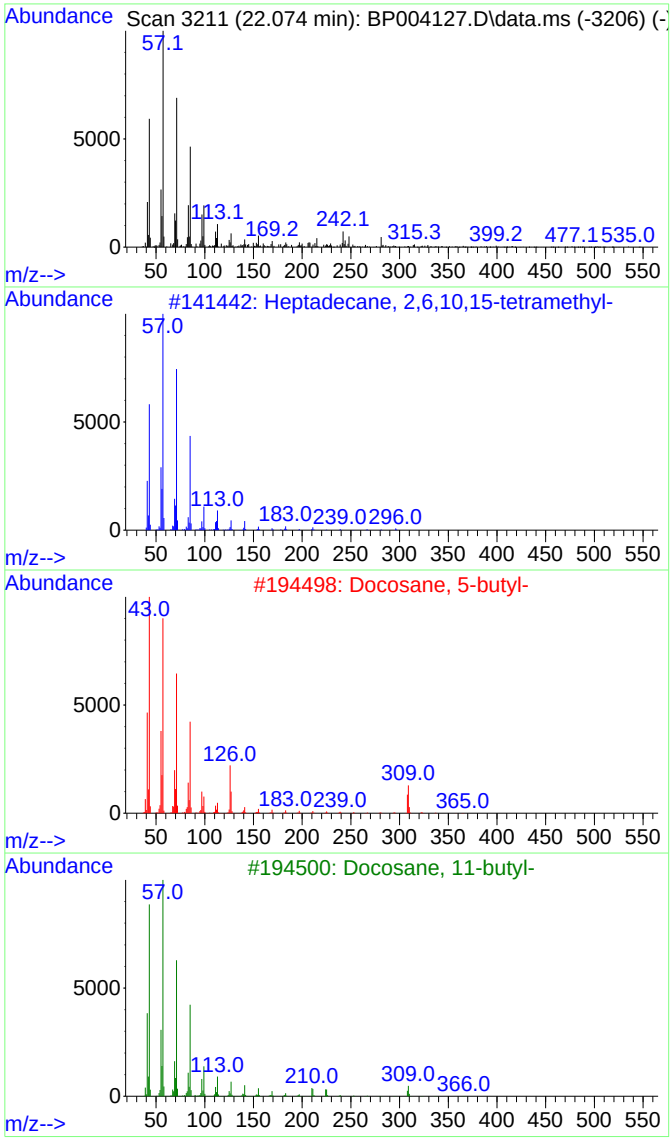
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

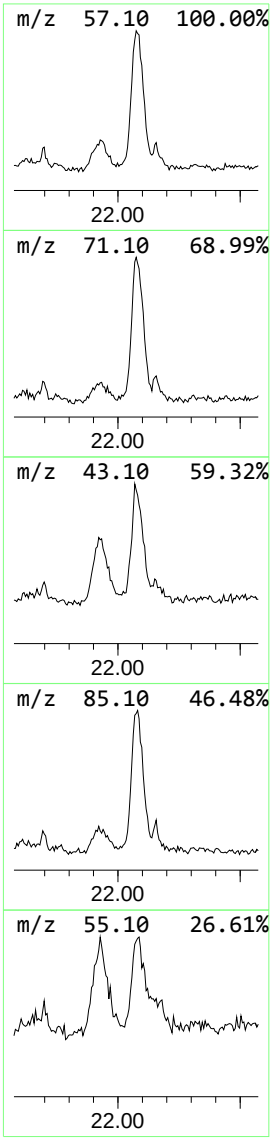
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.074	4.26 ng	328924	Chrysene-d12	21.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	97
2	Docosane, 5-butyl-	366	C26H54	055282-16-1	91
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90
5	Tetratriacontane, 17-hexadecyl-	703	C50H102	055256-07-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004127.D
Acq On : 02 Dec 2020 13:53
Operator : CG/JU
Sample : L4911-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SK-12-1-SPE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-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
Phenanthrene, 2...	18.410	2.0	ng	121541	4	17.563	1187950	20.0
3,5-Dimethoxy-4...	18.674	2.8	ng	164739	4	17.563	1187950	20.0
Desaspidinol	18.716	2.7	ng	161678	4	17.563	1187950	20.0
1-Heneicosyl fo...	21.257	7.8	ng	604502	5	21.598	1544440	20.0
.gamma.-Sitosterol	21.927	8.3	ng	643919	5	21.598	1544440	20.0
Heptadecane, 2,...	22.074	4.3	ng	328924	5	21.598	1544440	20.0