LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004128.D
Acq On : 02 Dec 2020 14:27
Operator : CG/JU
Sample : L4911-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

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: BP004128.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	340	344	351	rBV	43660	64689	1.51%	0.191%
2	5.734	427	433	449	rBV	1842083	2775335	64.71%	8.201%
3	7.381	704	713	728	rBV	1772210	2907000	67.78%	8.590%
4	8.193	844	851	858	rBV	472227	747304	17.43%	2.208%
5	9.357	1037	1049	1059	rBV	1108112	1805281	42.09%	5.334%
6	9.546	1074	1081	1097	rVB	51033	120587	2.81%	0.356%
7	11.022	1319	1332	1338	rBV	571422	977355	22.79%	2.888%
8	12.757	1622	1627	1637	rBV	20612	51483	1.20%	0.152%
9	13.445	1736	1744	1751	rBV	2349218	3389257	79.03%	10.015%
10	14.251	1876	1881	1887	rBV	114598	161084	3.76%	0.476%
11	14.545	1926	1931	1936	rBV	45134	67313	1.57%	0.199%
12	14.822	1972	1978	1984	rVV	818922	1155842	26.95%	3.415%
13	14.886	1984	1989	1995	rVB2	35461	54689	1.28%	0.162%
14	15.216	2040	2045	2052	rBV	37929	57025	1.33%	0.169%
15	15.863	2150	2155	2164	rVB2	79767	114065	2.66%	0.337%
16	16.310	2224	2231	2238	rBV	1790058	2534105	59.09%	7.488%
17	16.533	2266	2269	2275	rVB3	34842	46345	1.08%	0.137%
18	17.557	2437	2443	2447	rBV	954986	1342174	31.30%	3.966%
19	17.598	2447	2450	2457	rVV	550410	742371	17.31%	2.194%
20	17.692	2461	2466	2471	rVB	230416	322243	7.51%	0.952%
21	17.945	2505	2509	2514	rVB	76894	104072	2.43%	0.308%
22	18.410	2584	2588	2592	rBV	68108	92634	2.16%	0.274%
23	18.457	2592	2596	2602	rVB2	90295	121260	2.83%	0.358%
24	18.604	2615	2621	2624	rBV2	79988	152903	3.57%	0.452%
25	18.880	2664	2668	2671	rBV	46148	58939	1.37%	0.174%
26	18.922	2672	2675	2683	rVB	47623	66373	1.55%	0.196%
27	19.286	2733	2737	2742	rBV3	49944	98471	2.30%	0.291%
28	19.421	2757	2760	2768	rVB2	44505	68598	1.60%	0.203%
29	19.539	2775	2780	2786	rBV	701855	899697	20.98%	2.658%
30	19.857	2831	2834	2836	rBV2	103385	135223	3.15%	0.400%
31	19.892	2836	2840	2847	rVB	659745	872660	20.35%	2.579%
32	19.963	2848	2852	2853	rBV2	38535	50388	1.17%	0.149%
33	20.063	2864	2869	2875	rBV	3522200	4288688	100.00%	12.672%
34	20.121	2876	2879	2884	rVB	43217	53398	1.25%	0.158%
35	20.204	2889	2893	2898	rVB3	45737	85910	2.00%	0.254%
36	20.363	2918	2920	2924	rVB	86189	89902	2.10%	0.266%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004128.D
Acq On : 02 Dec 2020 14:27
Operator : CG/JU
Sample : L4911-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

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	20.457	2934	2936	2940	rVB	40164	44143	1.03%	0.130%
38	20.521	2944	2947	2950	rVB	64298	78445	1.83%	0.232%
39	20.657	2967	2970	2973	rBV	53973	69063	1.61%	0.204%
40	21.086	3040	3043	3049	rBV	96846	114825	2.68%	0.339%
41	21.257	3068	3072	3075	rBV2	293321	369102	8.61%	1.091%
42	21.327	3080	3084	3088	rBV2	196016	226215	5.27%	0.668%
43	21.368	3089	3091	3101	rVB	73818	111883	2.61%	0.331%
44	21.463	3103	3107	3116	rBV	519775	580362	13.53%	1.715%
45	21.598	3123	3130	3134	rBV2	1236490	2070308	48.27%	6.117%
46	21.633	3134	3136	3143	rVB	343834	430357	10.03%	1.272%
47	23.298	3413	3419	3424	rBV	346099	789198	18.40%	2.332%
48	23.821	3503	3508	3518	rVB	216738	439129	10.24%	1.298%
49	23.927	3521	3526	3534	rVB	195017	368118	8.58%	1.088%
50	24.039	3538	3545	3551	rBV	749711	1476806	34.43%	4.364%

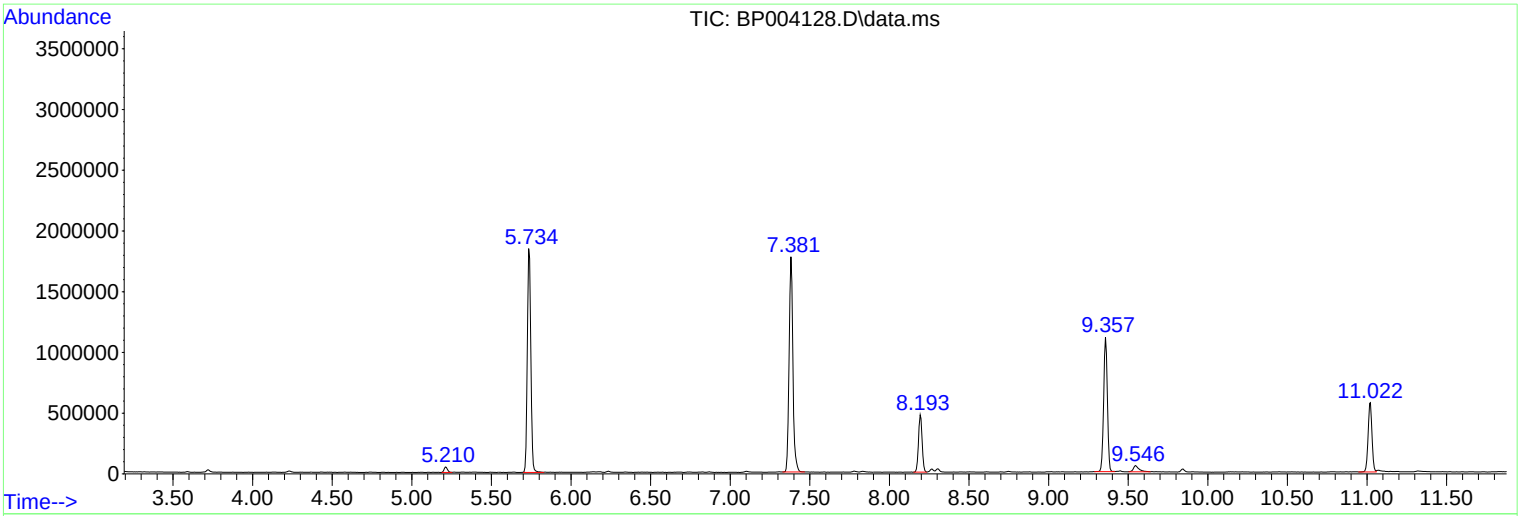
Sum of corrected areas: 33842617

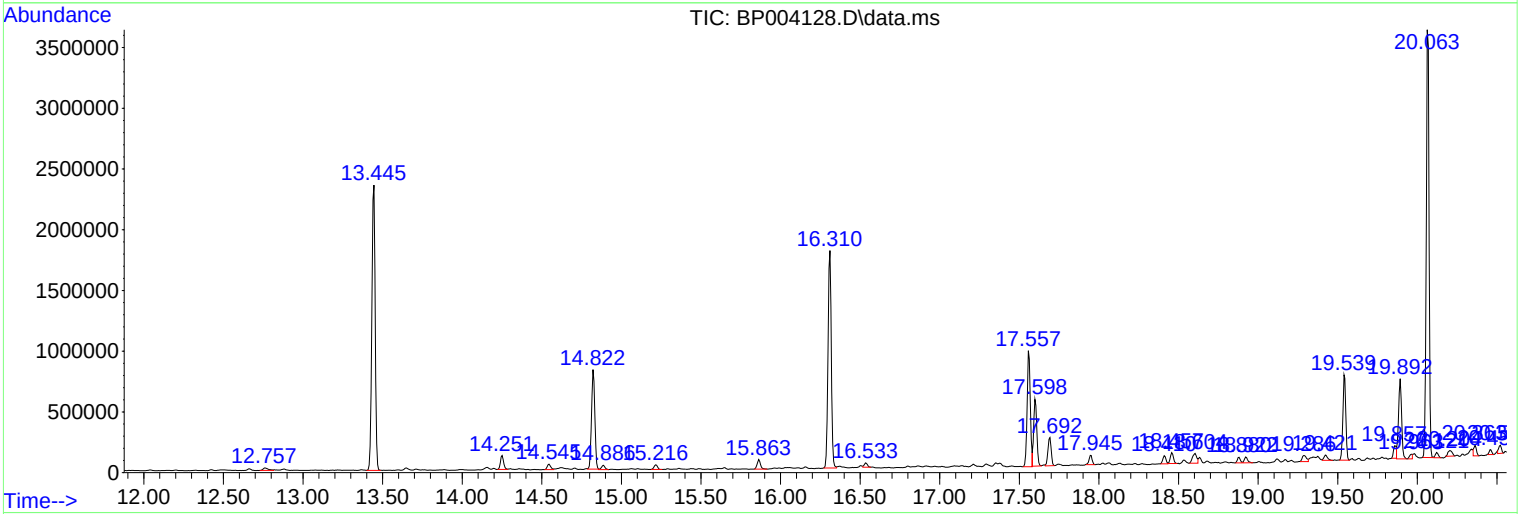
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004128.D
Acq On : 02 Dec 2020 14:27
Operator : CG/JU
Sample : L4911-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

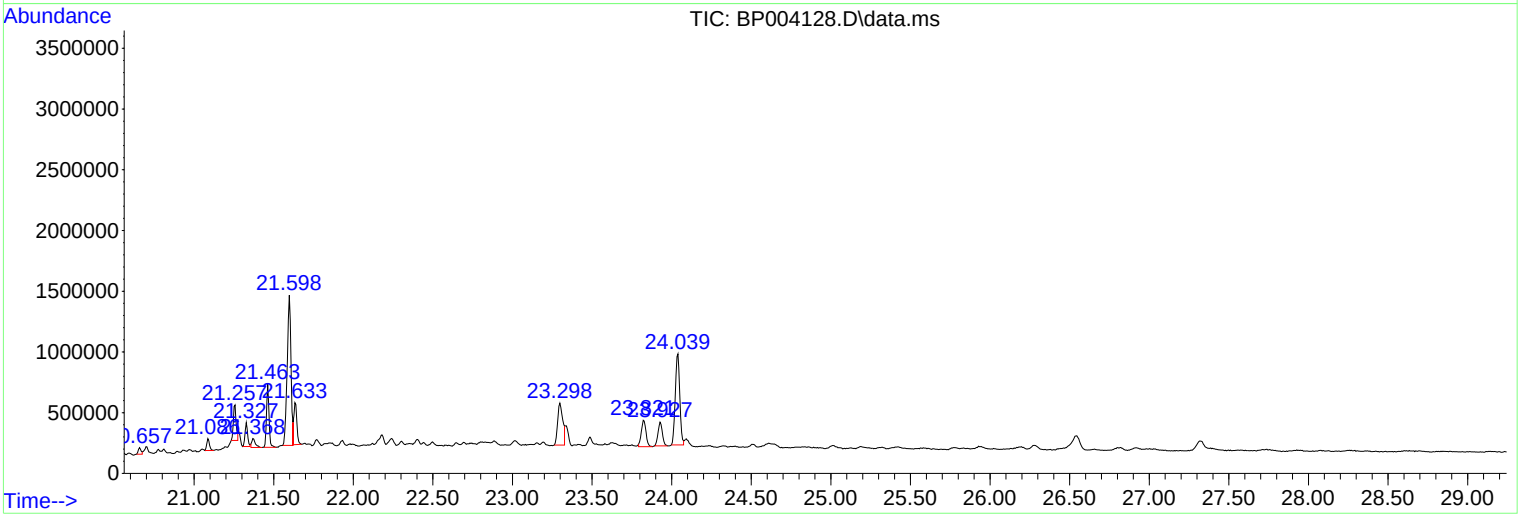
Instrument :
BNA_P
ClientSampleId :
SK-12-1-SPD

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 : BP004128.D
Acq On : 02 Dec 2020 14:27
Operator : CG/JU
Sample : L4911-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

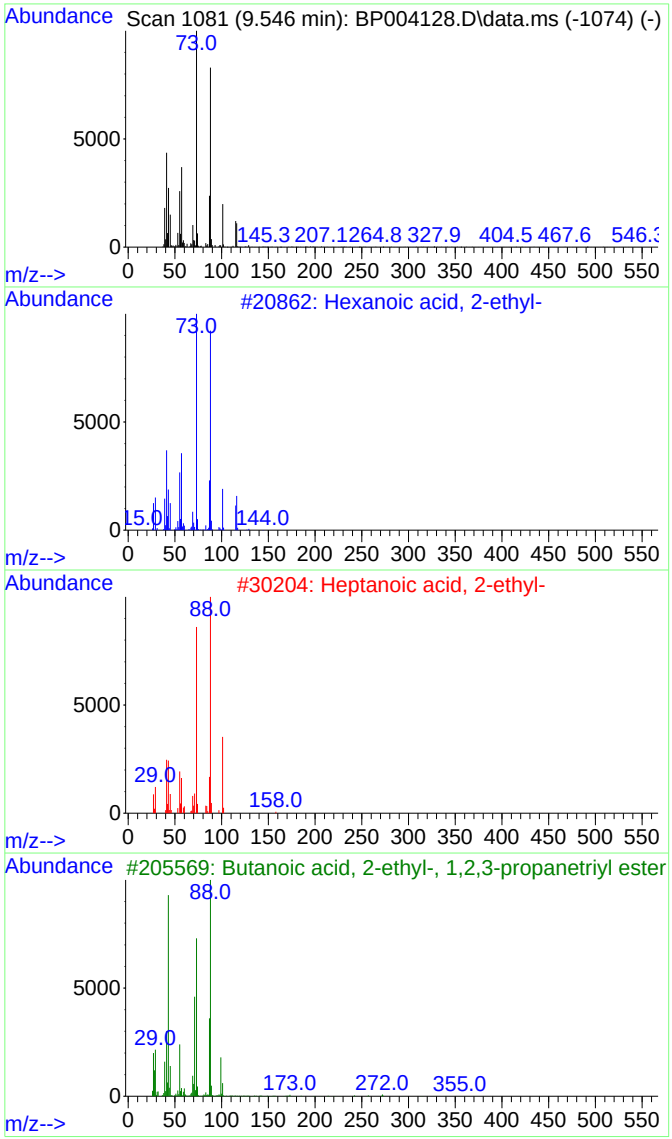
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

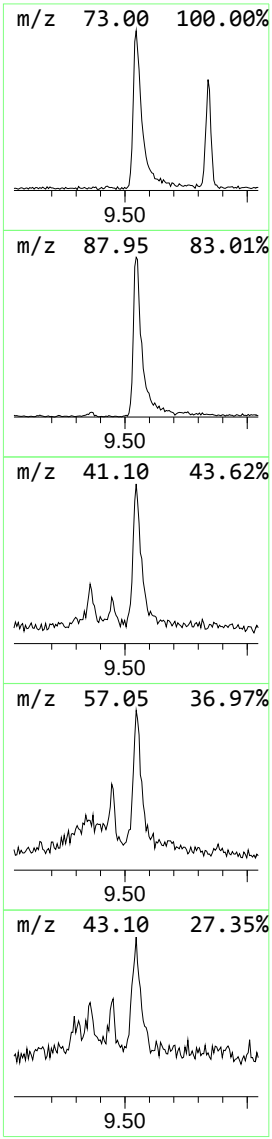
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.546	3.23 ng	120587	1,4-Dichlorobenzene-d4	8.193

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
4	Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	43
5	3-Aza-2-oxabicyclo[2.2.2]oct-5-e...	267	C10H12F3NO4	102698-35-1	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004128.D
Acq On : 02 Dec 2020 14:27
Operator : CG/JU
Sample : L4911-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

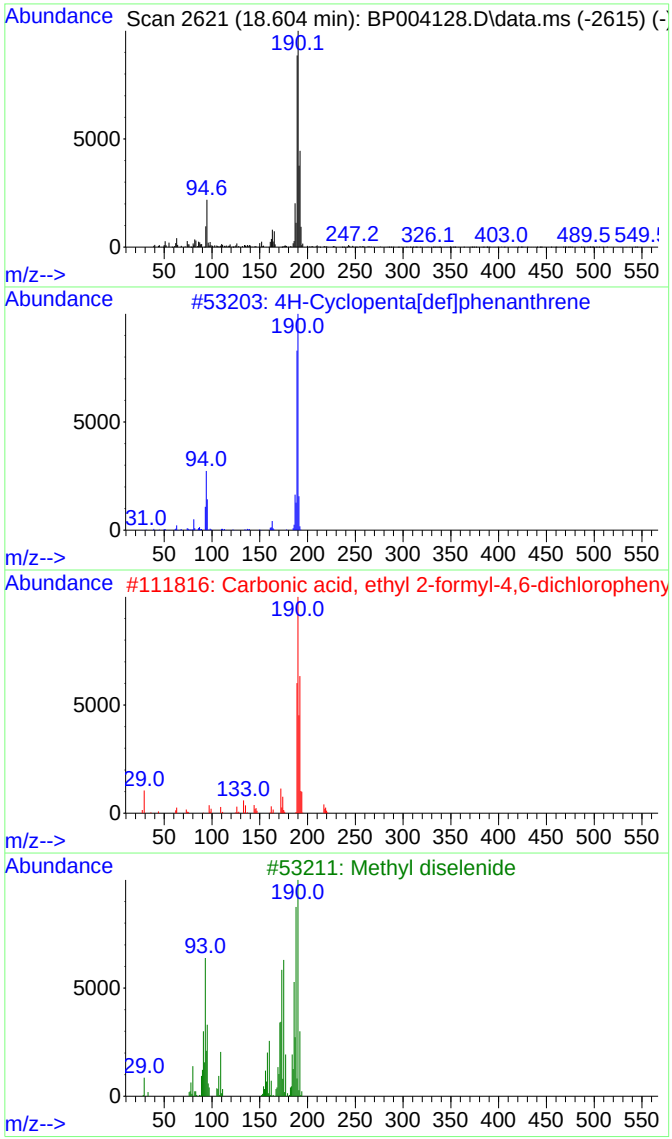
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

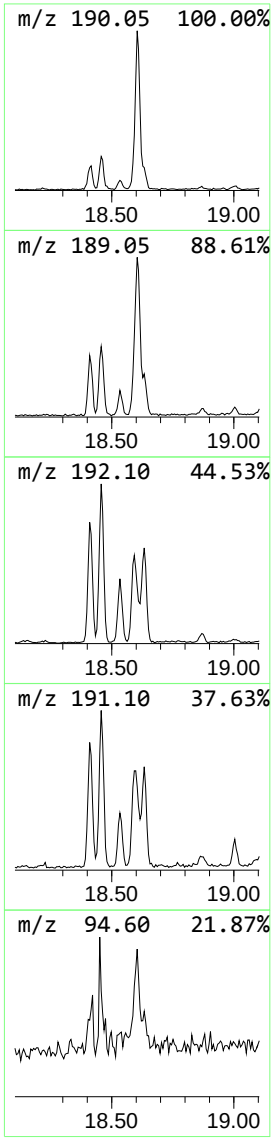
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.604	2.28 ng	152903	Phenanthrene-d10	17.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	1-Aminocyclopentanecarboxylic ac...	297	C11H17Cl2NO4	1000329-17-6	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004128.D
Acq On : 02 Dec 2020 14:27
Operator : CG/JU
Sample : L4911-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

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

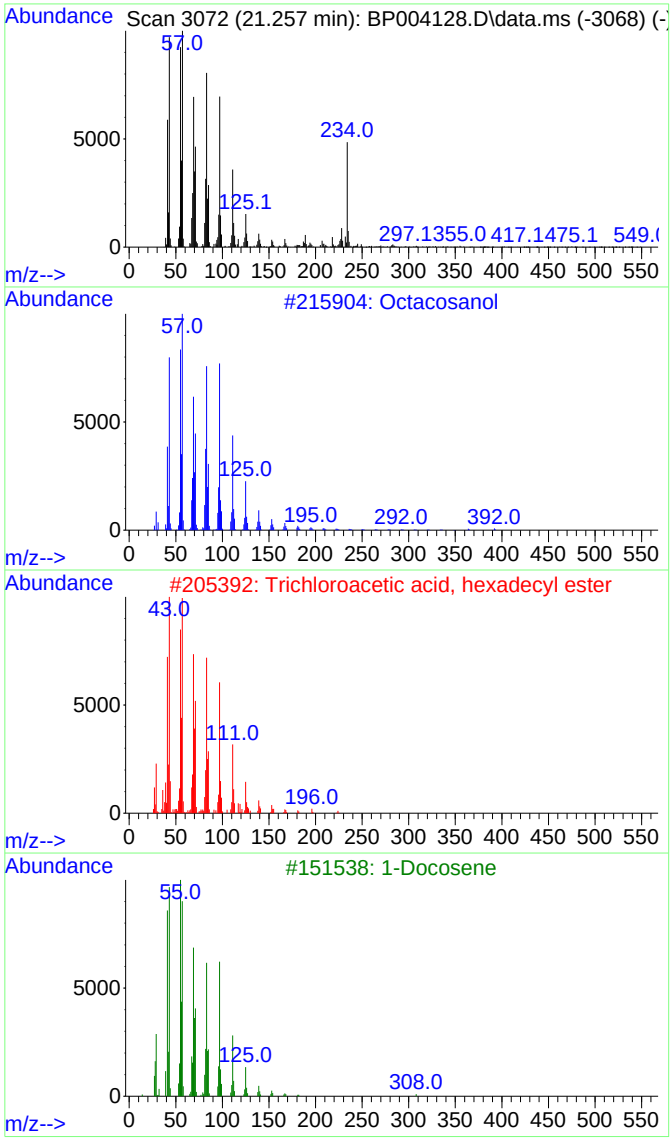
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

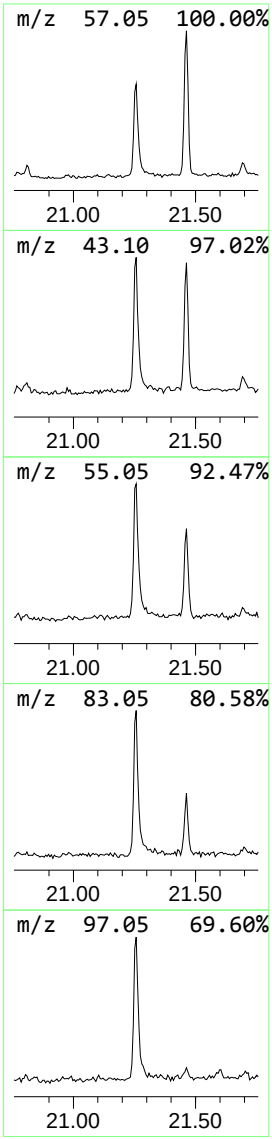
****

Peak Number 3 Octacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.257	3.57 ng	369102	Chrysene-d12	21.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	90
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3	1-Docosene	308	C22H44	001599-67-3	90
4	1-Heneicosanol	312	C21H44O	015594-90-8	89
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004128.D
Acq On : 02 Dec 2020 14:27
Operator : CG/JU
Sample : L4911-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

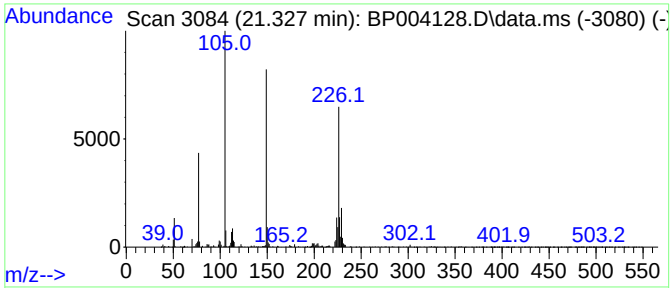
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

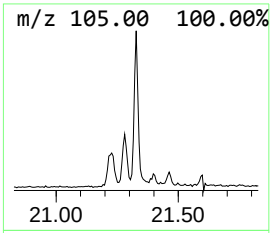
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

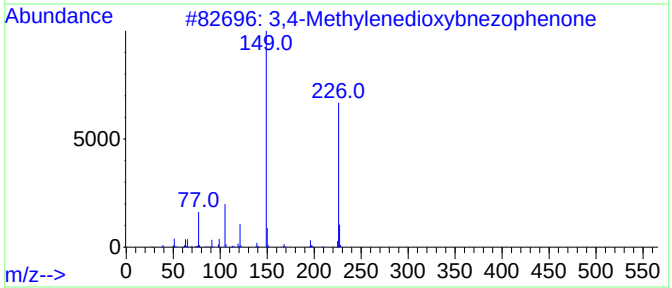
****
Peak Number 4 3,4-Methylenedioxybnezophenone Concentration Rank 5

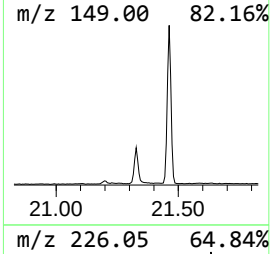
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.327	2.19 ng	226215	Chrysene-d12	21.598

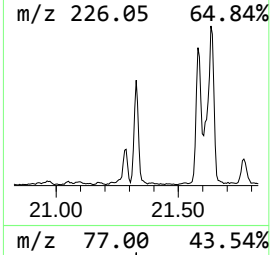
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Methylenedioxybnezophenone	226	C14H10O3	054225-86-4	53
2	Benzoic acid, 4-benzoyl-	226	C14H10O3	000611-95-0	50
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	47
4	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	47
5	Benzoic acid, 1-phenylethyl ester	226	C15H14O2	1000368-94-3	35

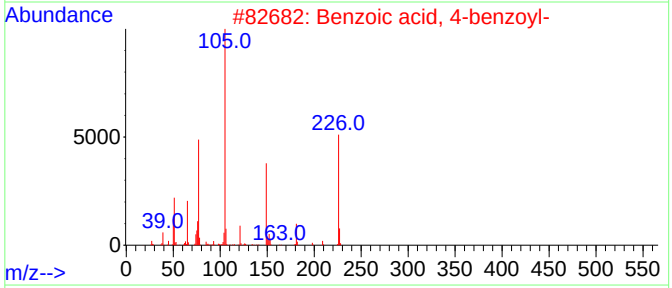


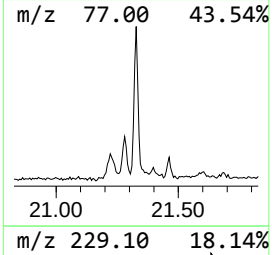


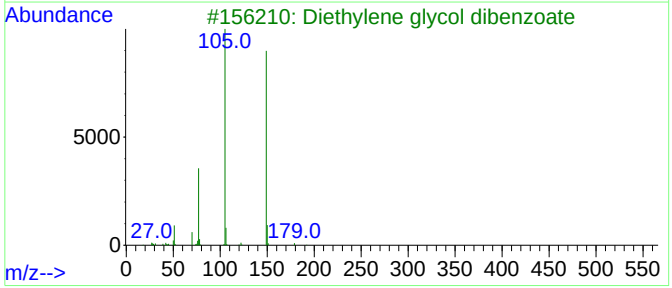


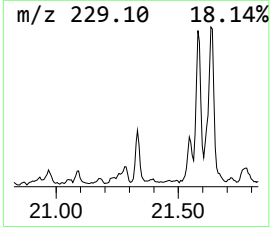












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004128.D
Acq On : 02 Dec 2020 14:27
Operator : CG/JU
Sample : L4911-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

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

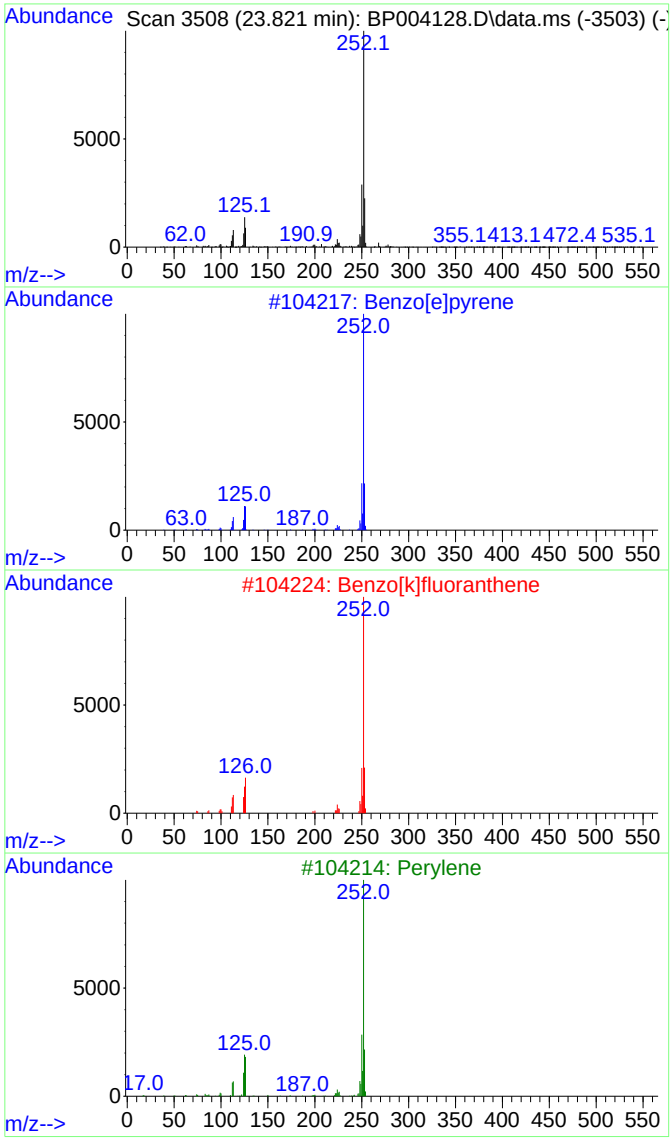
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

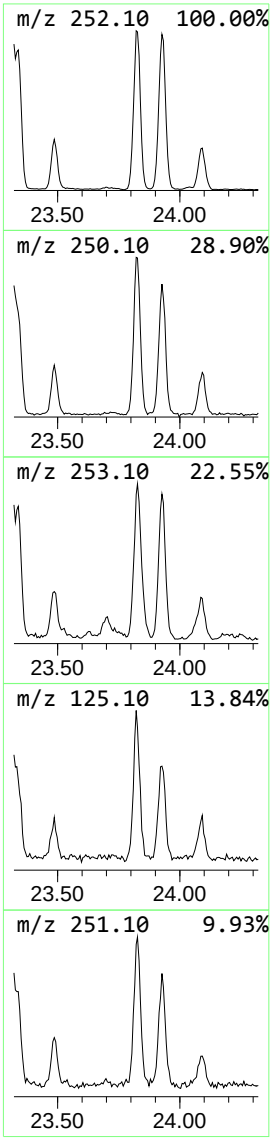
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.821	5.95 ng	439129	Perylene-d12	24.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Perylene	252	C20H12	000198-55-0	95
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004128.D
Acq On : 02 Dec 2020 14:27
Operator : CG/JU
Sample : L4911-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

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
Hexanoic acid, ...	9.546	3.2	ng	120587	1	8.193	747304	20.0
4H-Cyclopenta[d...	18.604	2.3	ng	152903	4	17.557	1342170	20.0
Octacosanol	21.257	3.6	ng	369102	5	21.598	2070310	20.0
3,4-Methylenedi...	21.327	2.2	ng	226215	5	21.598	2070310	20.0
Benzo[e]pyrene	23.821	6.0	ng	439129	6	24.039	1476810	20.0