LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092721\
Data File : BP007205.D
Acq On : 27 Sep 2021 14:59
Operator : CG/JU
Sample : M3943-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-TV-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\8270E-BP092121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007205.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.458	396	403	420	rBV	3219450	4734935	54.33%	7.675%
2	7.052	664	674	690	rBV	2900546	4823559	55.35%	7.819%
3	7.881	807	815	822	rBV	881838	1412788	16.21%	2.290%
4	9.040	1005	1012	1021	rBV	1851025	3125470	35.86%	5.066%
5	10.463	1247	1254	1272	rBV	1086261	1930814	22.16%	3.130%
6	10.681	1282	1291	1298	rBV	1135188	1865743	21.41%	3.024%
7	13.140	1700	1709	1720	rBV	4972052	7343747	84.27%	11.904%
8	13.416	1750	1756	1762	rBV	282363	434308	4.98%	0.704%
9	14.516	1933	1943	1950	rBV	1517358	2364299	27.13%	3.832%
10	14.910	2005	2010	2018	rBV4	59957	117817	1.35%	0.191%
11	16.004	2190	2196	2204	rVB	3789655	5261756	60.38%	8.529%
12	17.263	2404	2410	2414	rBV	1722655	2537972	29.12%	4.114%
13	17.304	2414	2417	2423	rVB	517227	718115	8.24%	1.164%
14	17.398	2428	2433	2438	rVB	112149	170413	1.96%	0.276%
15	17.933	2520	2524	2530	rBV	134893	171889	1.97%	0.279%
16	18.151	2553	2561	2563	rBV2	190090	360460	4.14%	0.584%
17	18.180	2563	2566	2570	rVB	144034	192010	2.20%	0.311%
18	18.322	2584	2590	2594	rBV2	147602	280721	3.22%	0.455%
19	18.357	2594	2596	2603	rVB	81270	88356	1.01%	0.143%
20	18.616	2636	2640	2643	rBV	71080	90223	1.04%	0.146%
21	19.016	2705	2708	2713	rBV	67187	140029	1.61%	0.227%
22	19.069	2713	2717	2722	rVB2	416842	493901	5.67%	0.801%
23	19.151	2728	2731	2735	rBV	63497	93831	1.08%	0.152%
24	19.198	2735	2739	2744	rVB	129031	156062	1.79%	0.253%
25	19.275	2747	2752	2758	rBV	1183813	1554561	17.84%	2.520%
26	19.627	2803	2812	2820	rBV	1200952	1833736	21.04%	2.972%
27	19.822	2839	2845	2850	rBV	6914327	8714639	100.00%	14.126%
28	19.945	2862	2866	2872	rBV4	67650	151062	1.73%	0.245%
29	20.104	2891	2893	2899	rVB2	143013	214625	2.46%	0.348%
30	20.210	2908	2911	2914	rBV2	81736	97802	1.12%	0.159%
31	20.263	2918	2920	2924	rVB	87287	96512	1.11%	0.156%
32	20.445	2948	2951	2954	rVB2	106215	120004	1.38%	0.195%
33	21.063	3053	3056	3064	rVB4	368145	545041	6.25%	0.883%
34	21.351	3099	3105	3109	rBV2	2264013	3619246	41.53%	5.866%
35	21.386	3109	3111	3118	rVB	573123	648705	7.44%	1.051%
36	22.457	3290	3293	3300	rVB2	244549	342736	3.93%	0.556%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092721\
Data File : BP007205.D
Acq On : 27 Sep 2021 14:59
Operator : CG/JU
Sample : M3943-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-TV-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\8270E-BP092121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.027	3385	3390	3396	rBV	484169	1158386	13.29%	1.878%
38	23.651	3492	3496	3504	rVB	457149	881466	10.11%	1.429%
39	23.763	3509	3515	3522	rVV2	1390898	2806250	32.20%	4.549%

Sum of corrected areas: 61693989

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092721\
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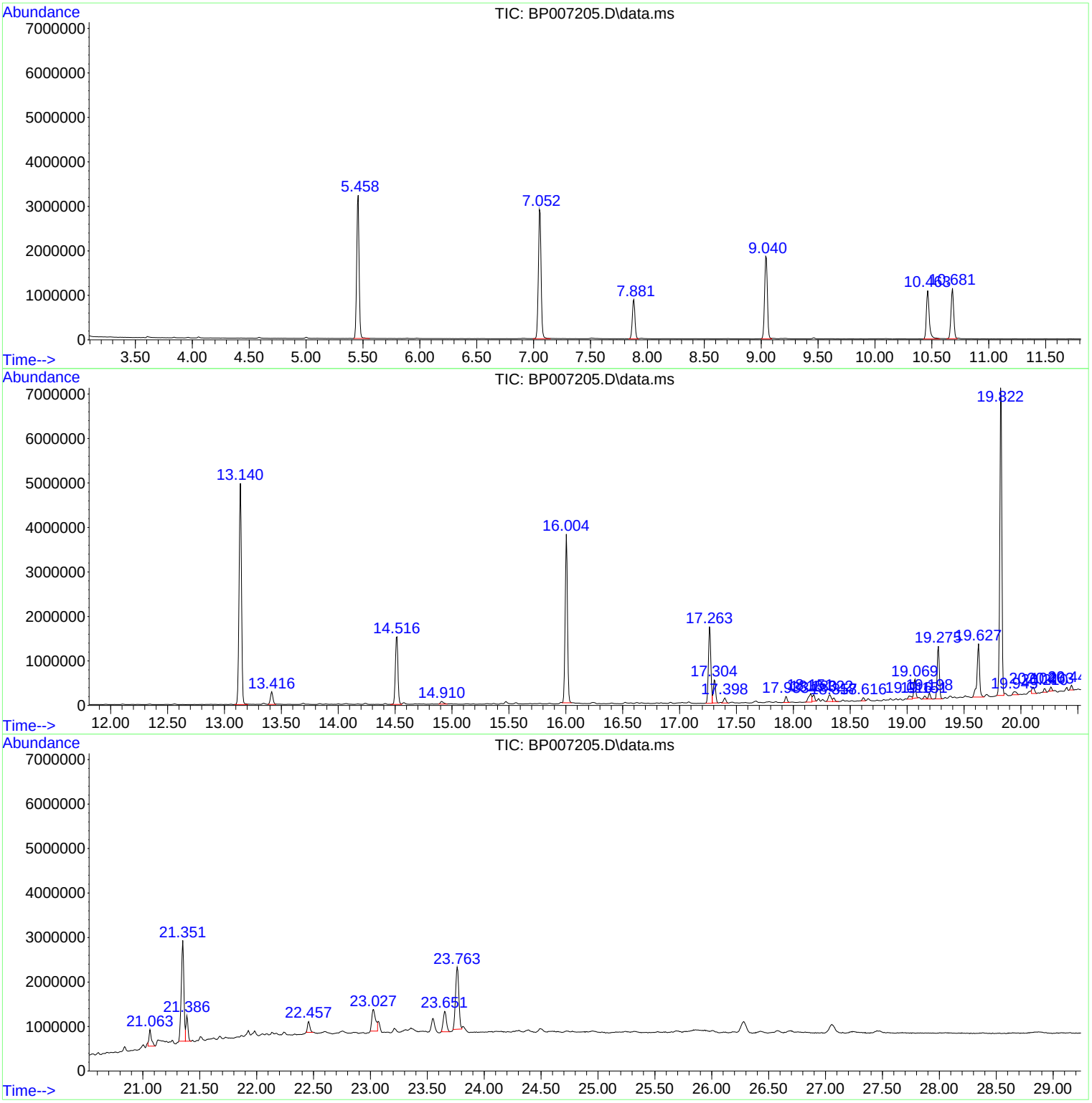
Acq On : 27 Sep 2021 14:59
Operator : CG/JU
Sample : M3943-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-TV-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092721\
Data File : BP007205.D
Acq On : 27 Sep 2021 14:59
Operator : CG/JU
Sample : M3943-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-TV-1

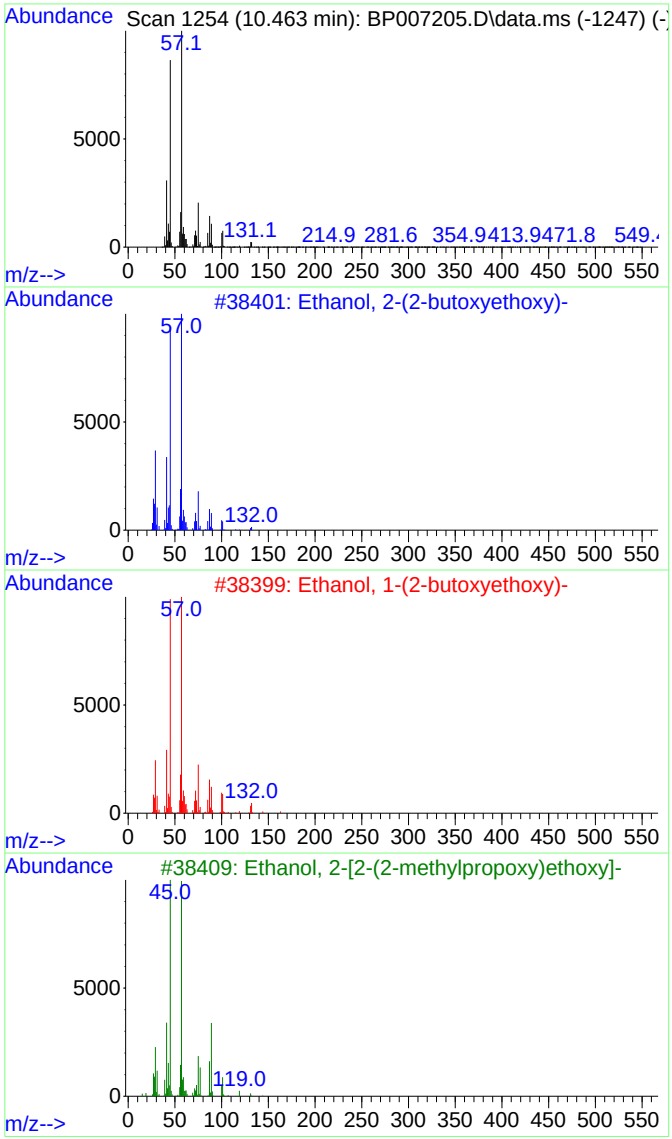
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

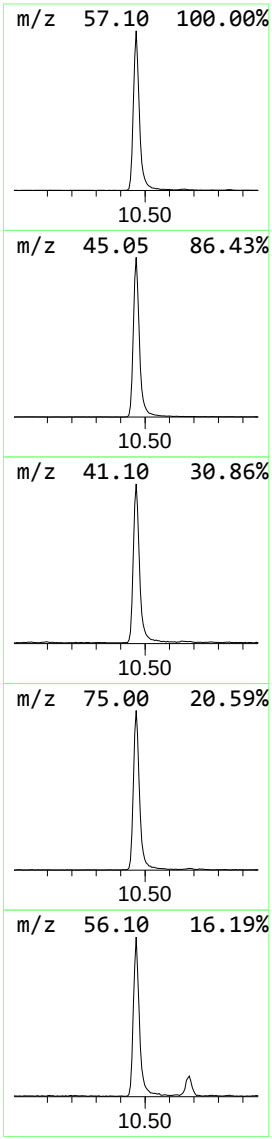
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.463	20.70 ng	1930810	Naphthalene-d8	10.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092721\
Data File : BP007205.D
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Operator : CG/JU
Sample : M3943-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-TV-1

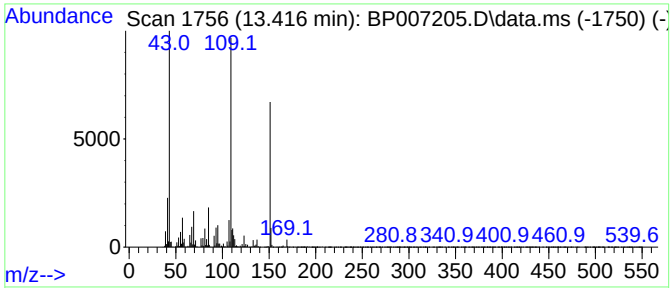
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

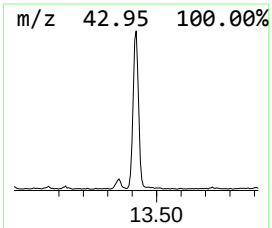
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

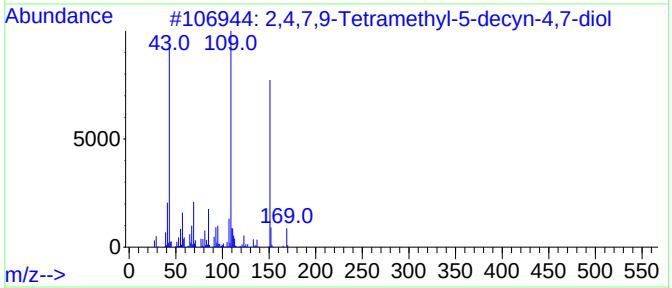
****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

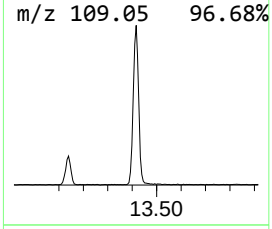
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.416	3.67 ng	434308	Acenaphthene-d10	14.516

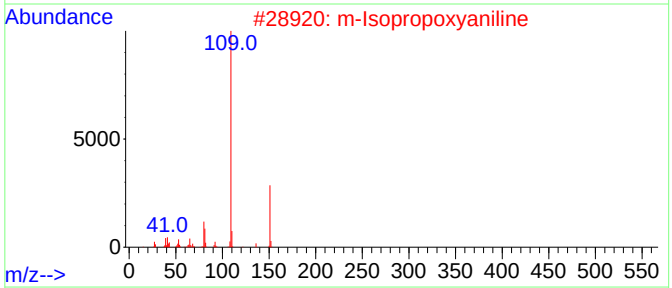
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
3	Metacetamol	151	C8H9NO2	000621-42-1	53
4	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	50
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	42

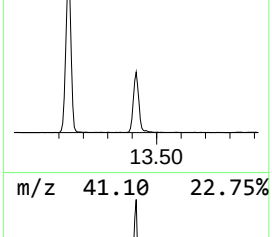


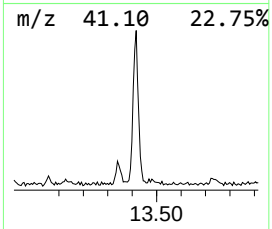


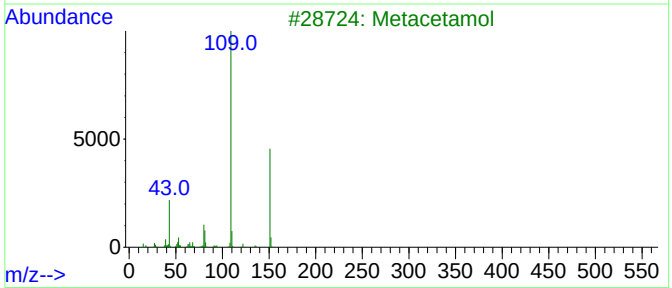


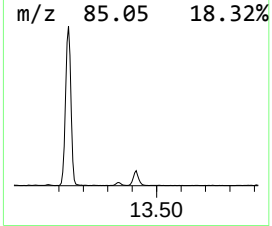












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092721\
Data File : BP007205.D
Acq On : 27 Sep 2021 14:59
Operator : CG/JU
Sample : M3943-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-TV-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

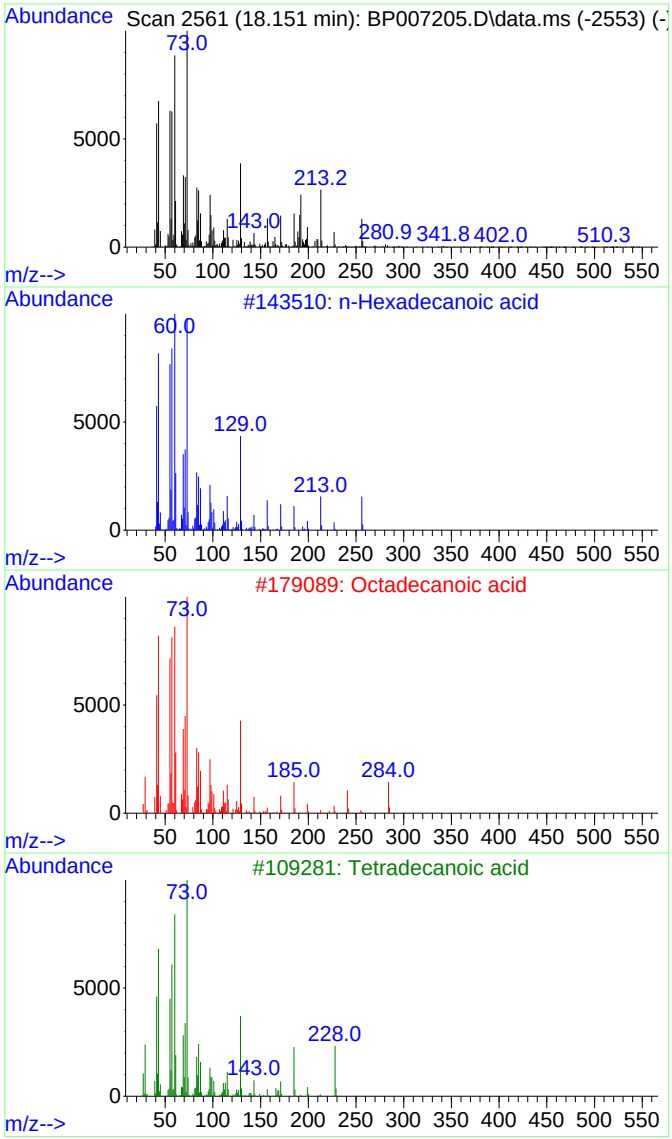
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

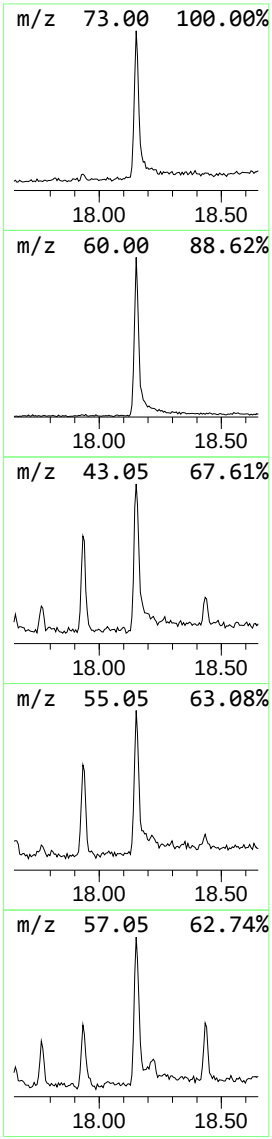
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	2.84 ng	360460	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092721\
Data File : BP007205.D
Acq On : 27 Sep 2021 14:59
Operator : CG/JU
Sample : M3943-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-TV-1

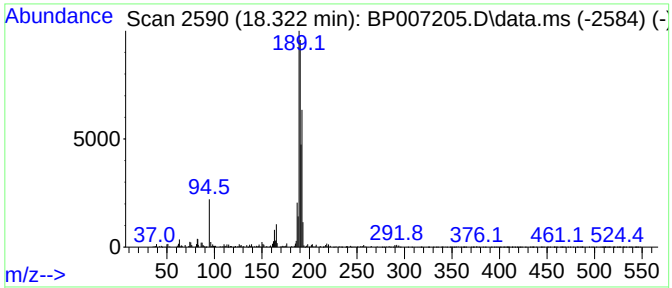
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

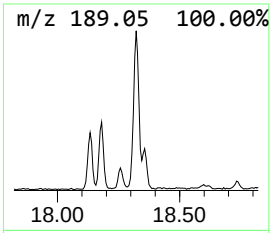
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

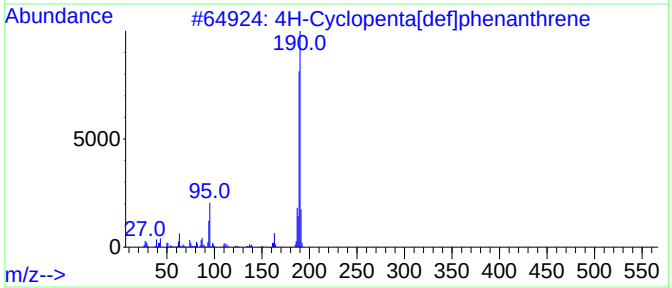
****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

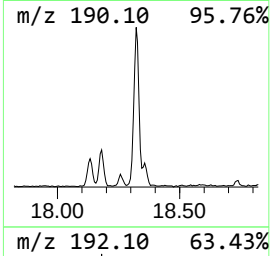
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.322	2.21 ng	280721	Phenanthrene-d10	17.263

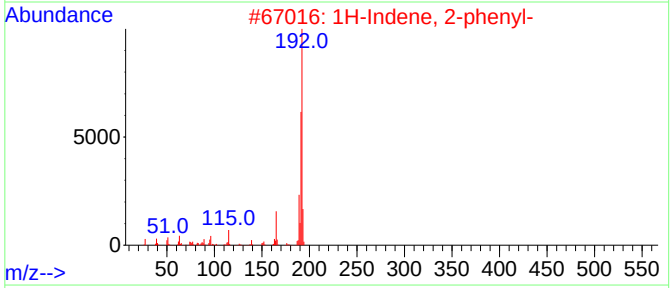
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	30
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	25
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	25
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	18

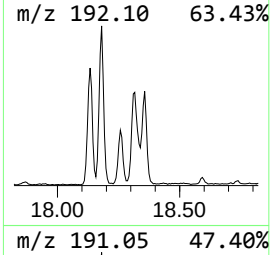


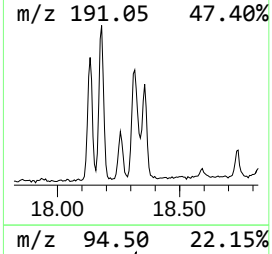


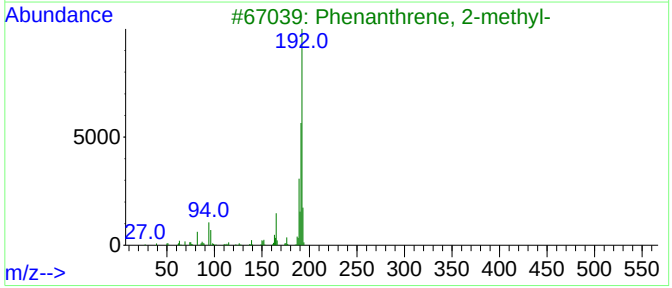


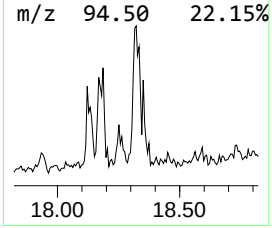












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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WC-TV-1

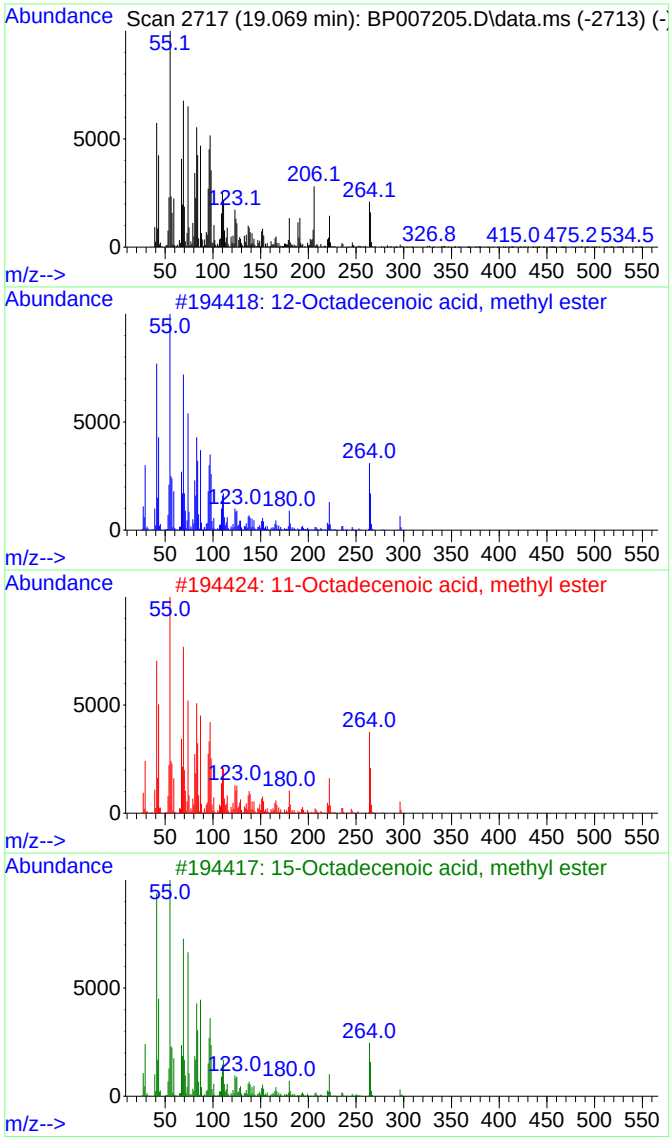
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

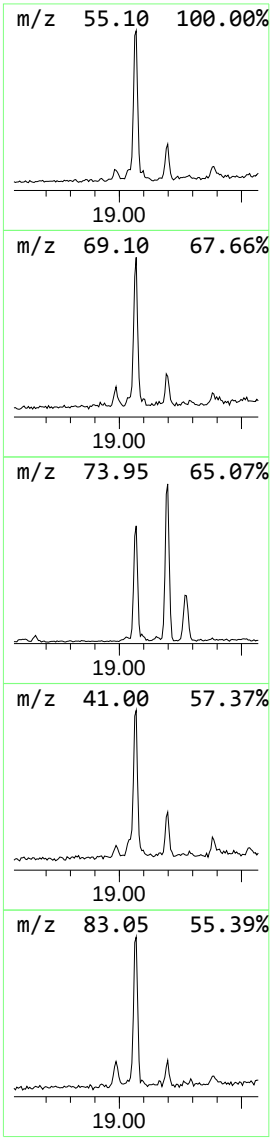
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 12-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.069	3.89 ng	493901	Phenanthrene-d10	17.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	97
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	95
5	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	95





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Data File : BP007205.D
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Operator : CG/JU
Sample : M3943-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-TV-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

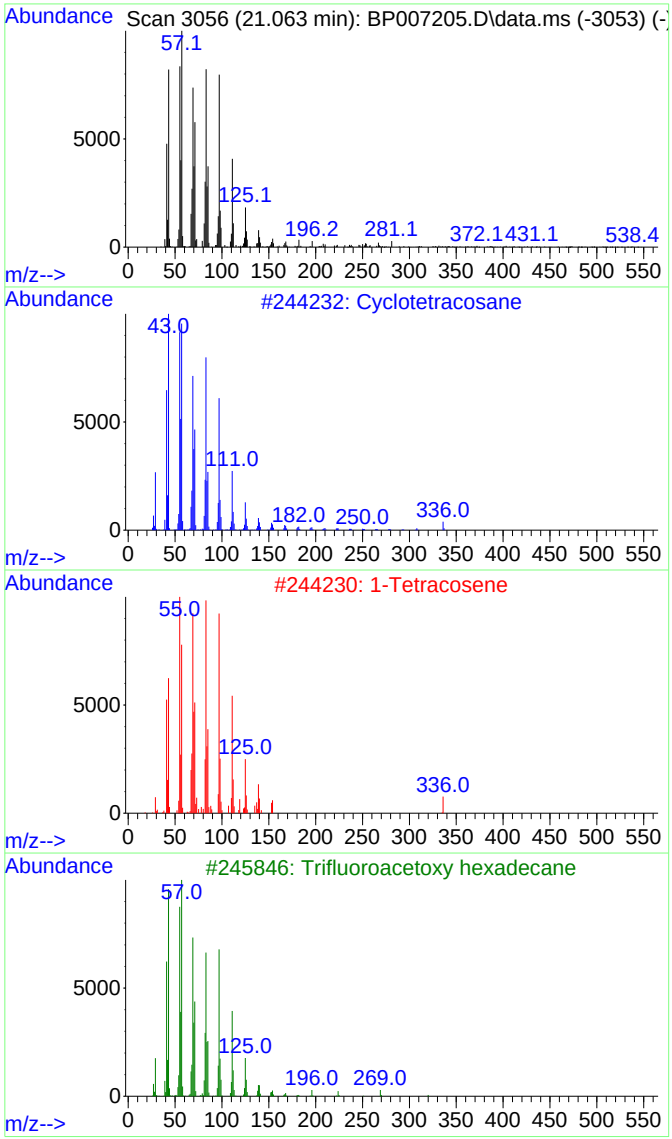
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

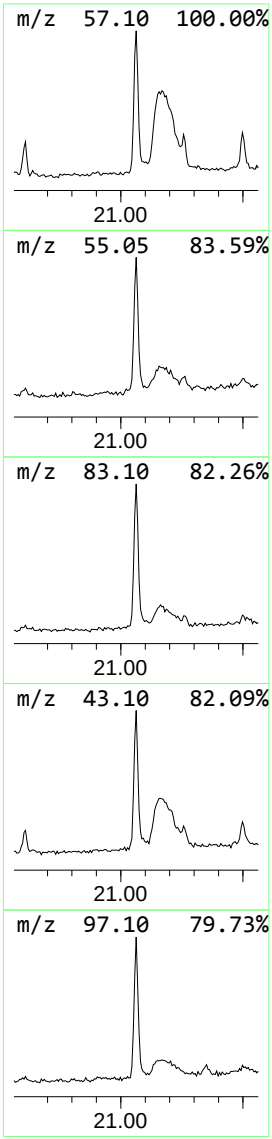
****

Peak Number 6 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.063	3.01 ng	545041	Chrysene-d12	21.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	99
2	1-Tetracosene	336	C24H48	010192-32-2	99
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Nonacos-1-ene	406	C29H58	018835-35-3	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092721\
Data File : BP007205.D
Acq On : 27 Sep 2021 14:59
Operator : CG/JU
Sample : M3943-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WC-TV-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.463	20.7	ng	1930810	2	10.681	1865740	20.0
2,4,7,9-Tetrame...	13.416	3.7	ng	434308	3	14.516	2364300	20.0
n-Hexadecanoic ...	18.151	2.8	ng	360460	4	17.263	2537970	20.0
4H-Cyclopenta[d...	18.322	2.2	ng	280721	4	17.263	2537970	20.0
12-Octadecenoic...	19.069	3.9	ng	493901	4	17.263	2537970	20.0
Cyclotetracosane	21.063	3.0	ng	545041	5	21.351	3619250	20.0