LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008422.D
Acq On : 15 Dec 2021 18:08
Operator : CG/JU
Sample : M5017-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP1

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-BP121421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008422.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	316	321	330	rBV	114272	158493	6.78%	1.028%
2	5.340	395	400	418	rBV	754839	1212352	51.83%	7.864%
3	6.940	666	672	692	rBV	650569	1204588	51.50%	7.813%
4	7.740	802	808	818	rVB	197239	316502	13.53%	2.053%
5	8.910	998	1007	1030	rBV	409226	770175	32.93%	4.996%
6	10.540	1277	1284	1300	rBV	210392	401057	17.15%	2.601%
7	13.016	1698	1705	1719	rBV	981437	1511635	64.63%	9.805%
8	14.398	1933	1940	1947	rBV	316651	500957	21.42%	3.249%
9	15.904	2188	2196	2214	rBV	715726	1212306	51.83%	7.864%
10	17.163	2403	2410	2414	rBV	377017	591167	25.27%	3.835%
11	17.204	2414	2417	2424	rVB	88464	131620	5.63%	0.854%
12	17.298	2429	2433	2440	rVB2	19913	34765	1.49%	0.226%
13	17.581	2473	2481	2488	rBV2	19706	45220	1.93%	0.293%
14	18.063	2560	2563	2572	rVB3	43470	79185	3.39%	0.514%
15	18.222	2586	2590	2594	rBV3	16600	27199	1.16%	0.176%
16	18.516	2637	2640	2644	rBV	17127	24706	1.06%	0.160%
17	18.575	2645	2650	2658	rVV	142668	198515	8.49%	1.288%
18	19.075	2729	2735	2740	rBV	33122	53671	2.29%	0.348%
19	19.180	2747	2753	2761	rBV	397974	562171	24.03%	3.646%
20	19.533	2809	2813	2822	rVB	288008	394100	16.85%	2.556%
21	19.733	2841	2847	2862	rVB	1887308	2338987	100.00%	15.172%
22	20.763	3018	3022	3027	rBV	55581	80167	3.43%	0.520%
23	20.980	3055	3059	3066	rVB4	107912	197445	8.44%	1.281%
24	21.057	3069	3072	3077	rVV	42697	52837	2.26%	0.343%
25	21.263	3102	3107	3111	rBV	611248	891401	38.11%	5.782%
26	21.304	3111	3114	3120	rVB	127150	161845	6.92%	1.050%
27	21.380	3122	3127	3139	rBV	1017483	1367670	58.47%	8.871%
28	23.633	3504	3510	3519	rVB2	455698	896112	38.31%	5.813%

Sum of corrected areas: 15416848

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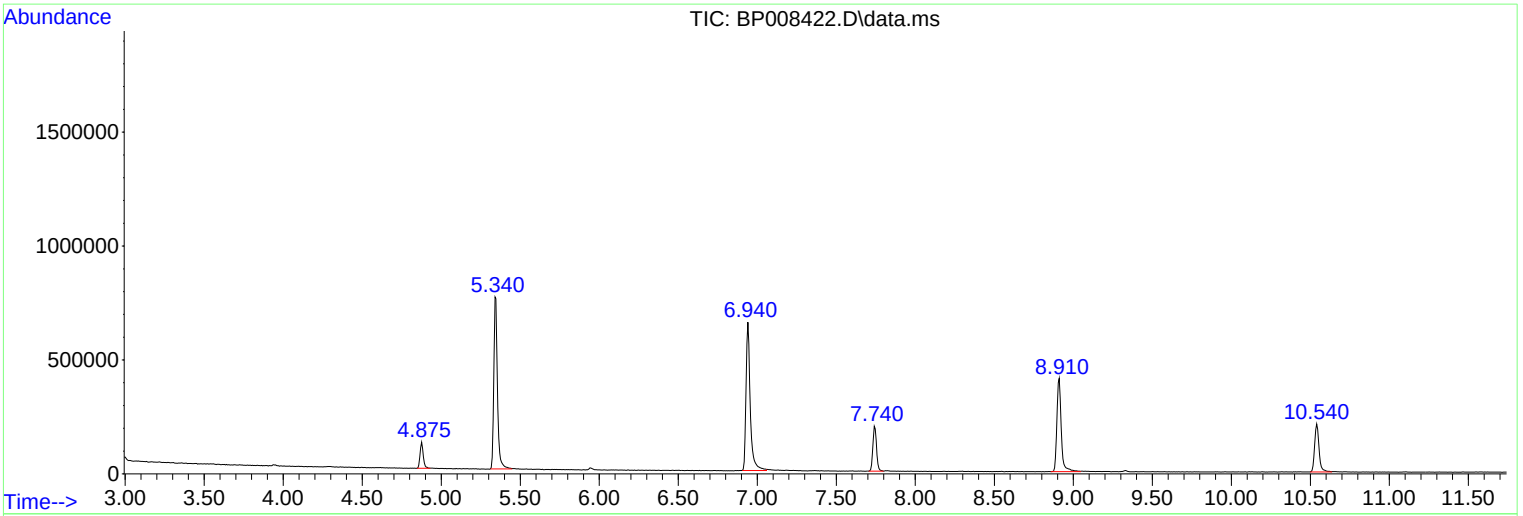
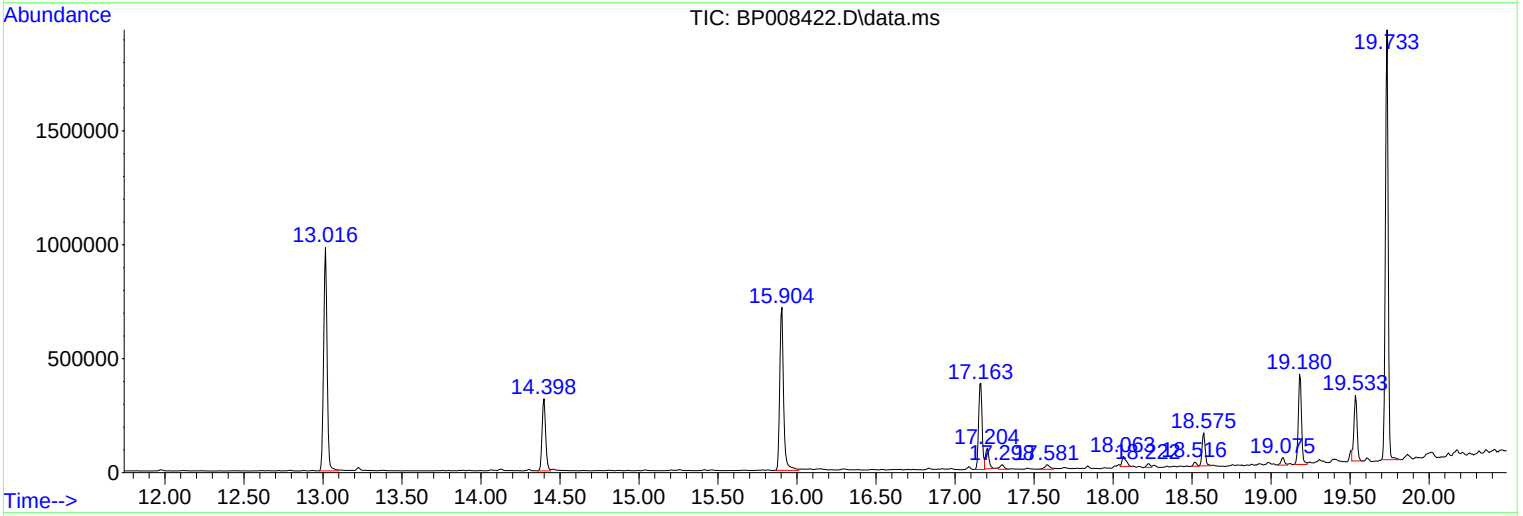
Misc :
ALS Vial : 15 Sample Multiplier: 1

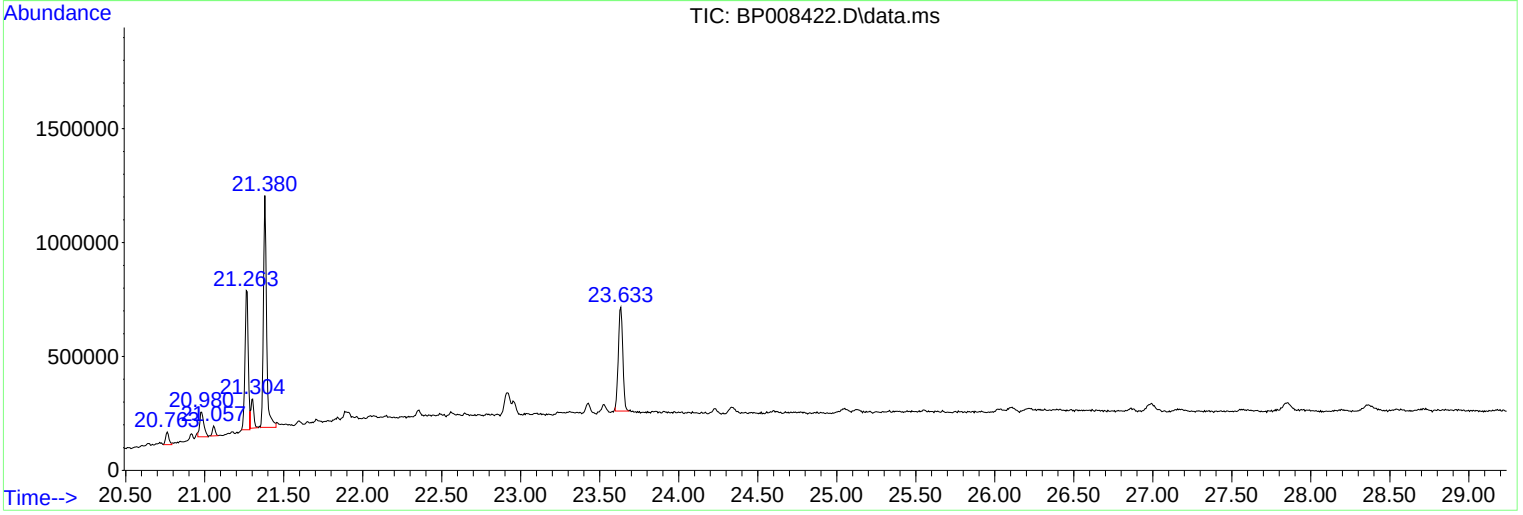
Instrument :
BNA_P
ClientSampleId :
TP1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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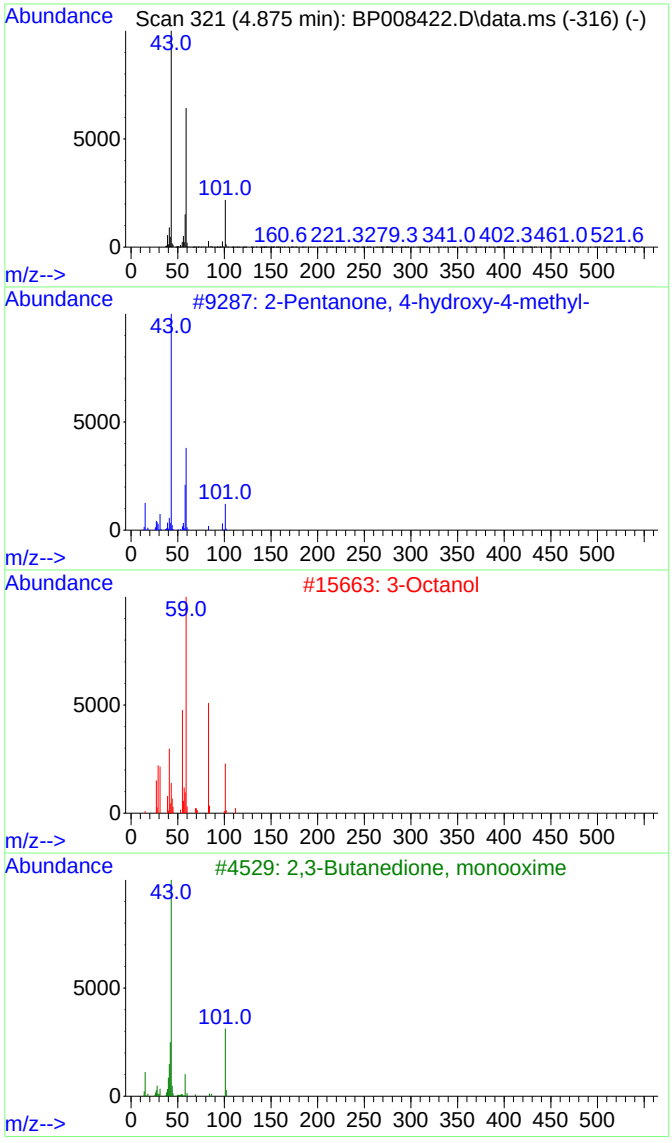
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

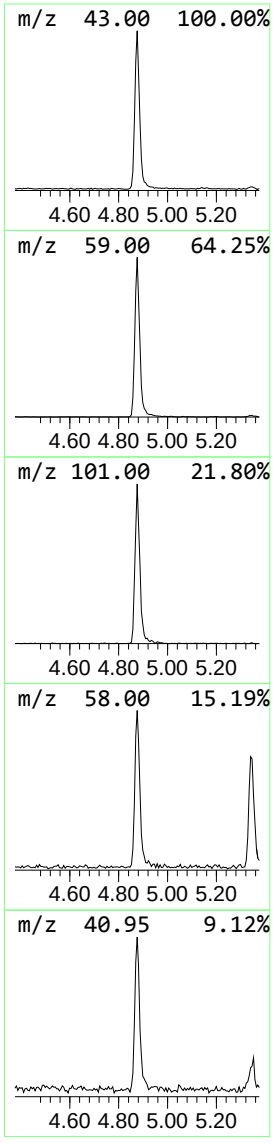
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	10.02 ng	158493	1,4-Dichlorobenzene-d4	7.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Octanol	130	C8H18O	000589-98-0	36
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17





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Data File : BP008422.D
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Operator : CG/JU
Sample : M5017-09
Misc :
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Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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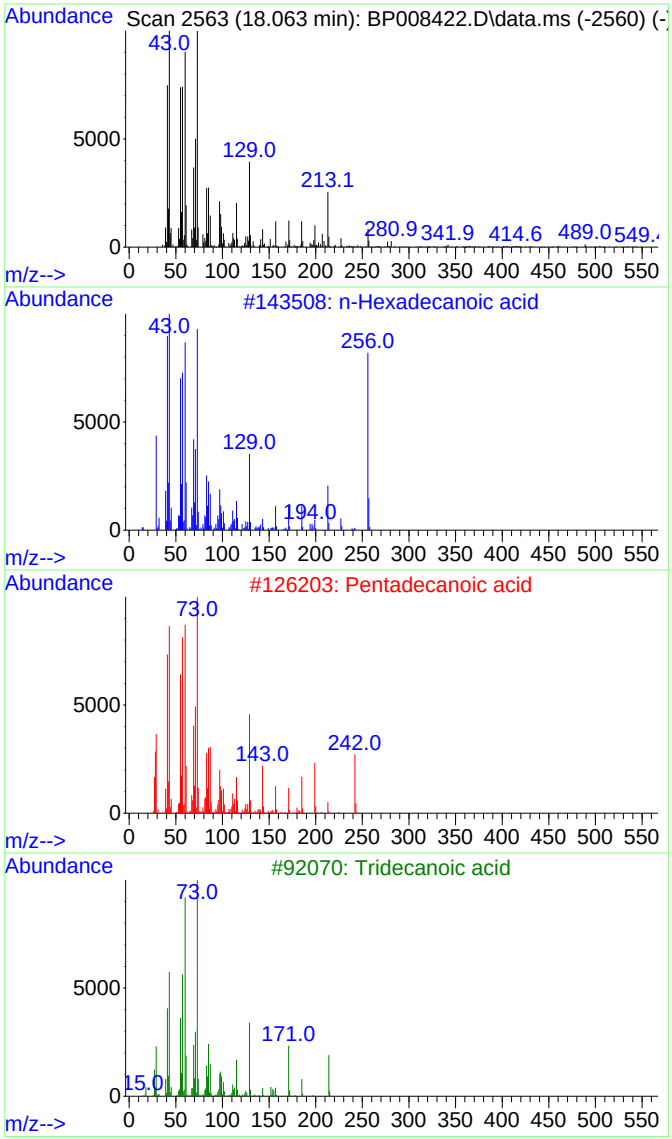
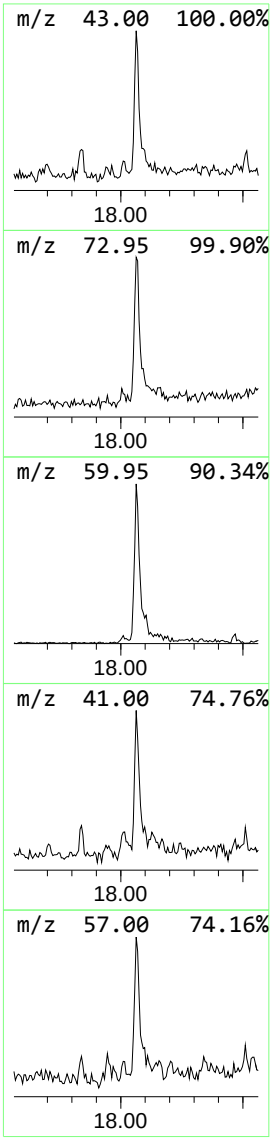
Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	2.68 ng	79185	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121521\
Data File : BP008422.D
Acq On : 15 Dec 2021 18:08
Operator : CG/JU
Sample : M5017-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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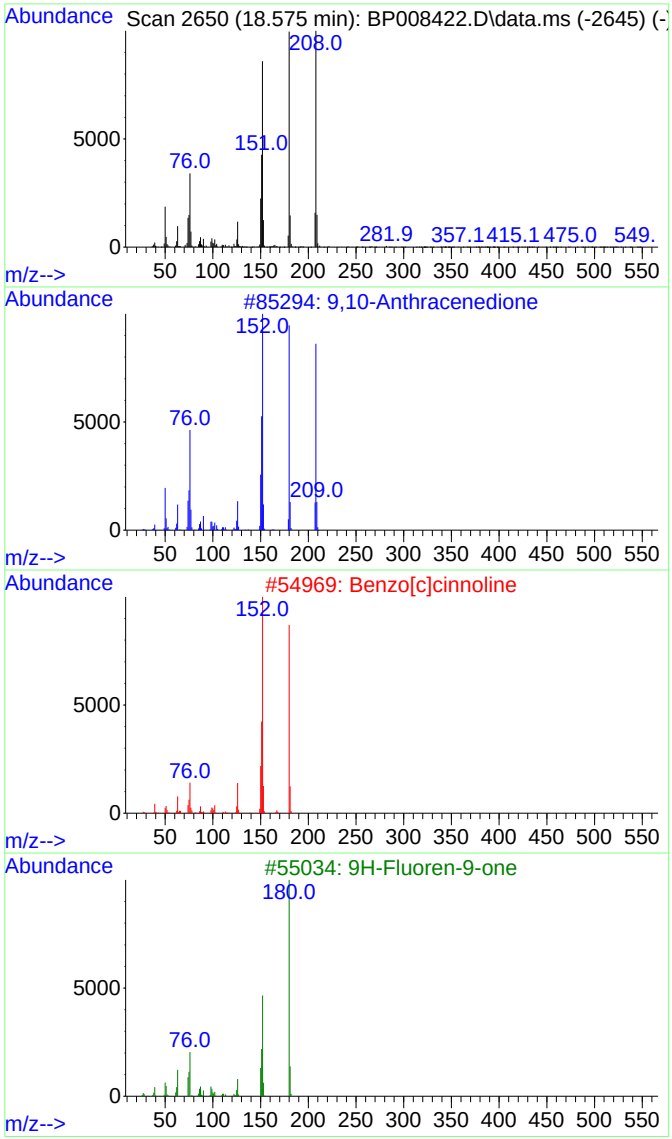
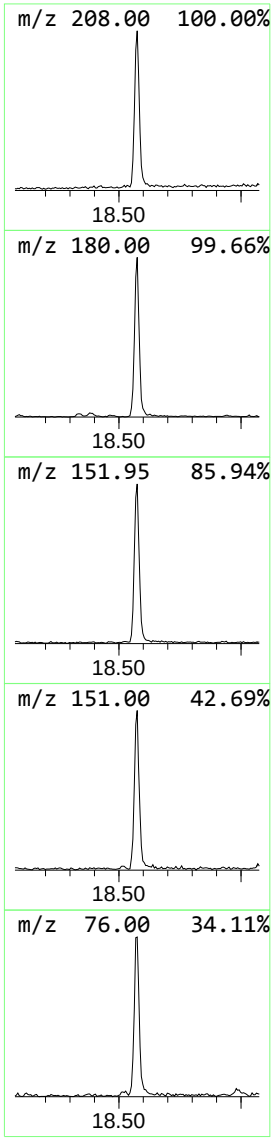
Peak Number 3 9,10-Anthracenedione Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.575	6.72 ng	198515	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	98
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	96
3	9H-Fluoren-9-one	180	C13H8O	000486-25-9	70
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	64
5	1,4-Anthracenedione	208	C14H8O2	000635-12-1	53





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Acq On : 15 Dec 2021 18:08
Operator : CG/JU
Sample : M5017-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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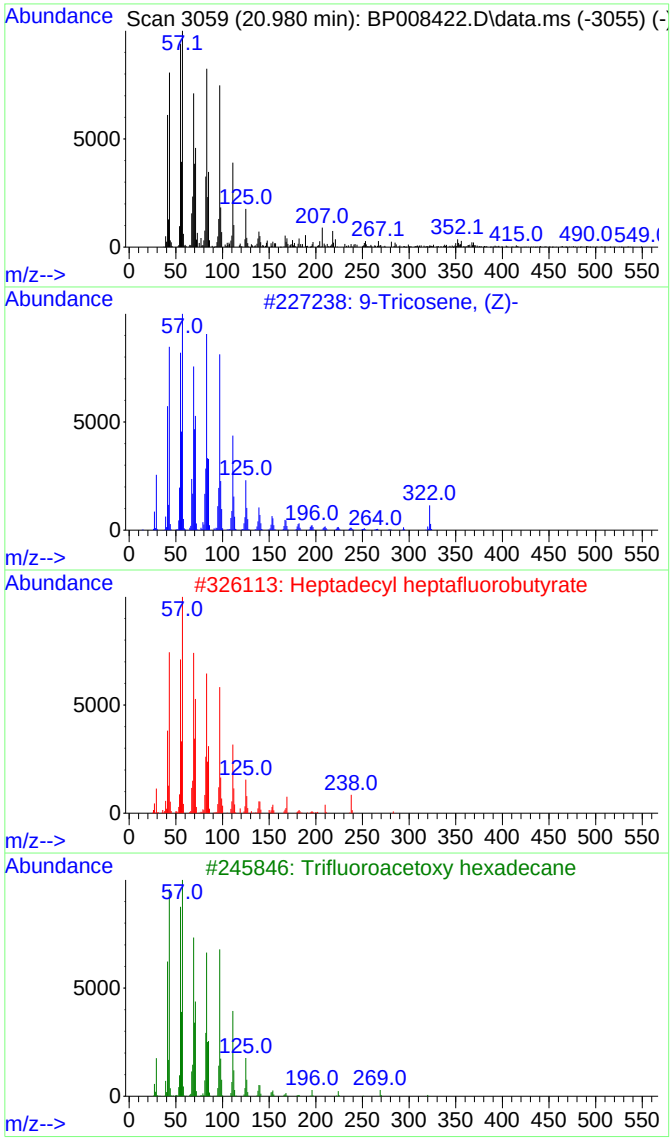
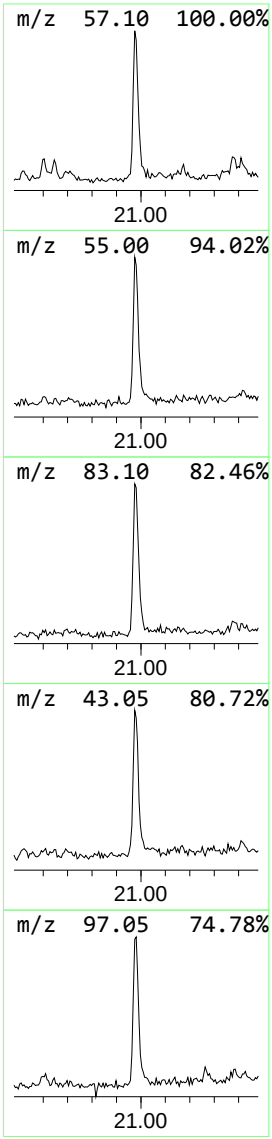
Peak Number 4 9-Tricosene, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	4.43 ng	197445	Chrysene-d12	21.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91





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Data File : BP008422.D
Acq On : 15 Dec 2021 18:08
Operator : CG/JU
Sample : M5017-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

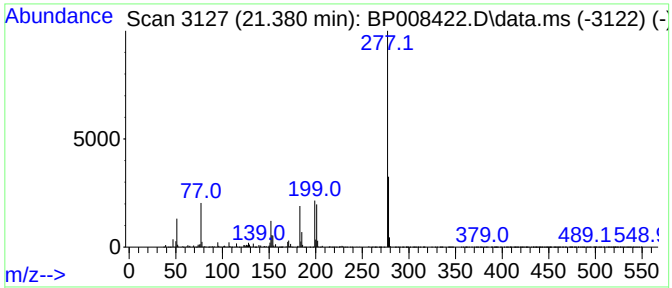
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

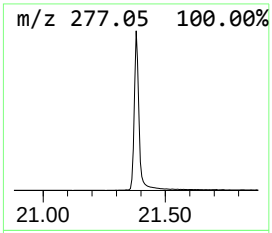
****

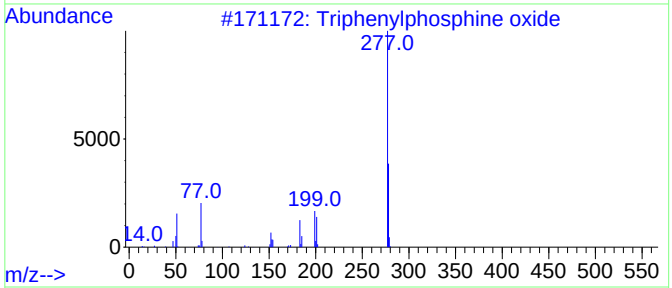
Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

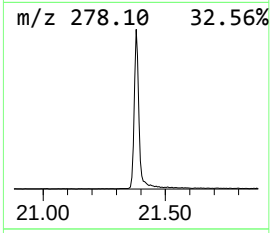
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.380	30.69 ng	1367670	Chrysene-d12	21.263

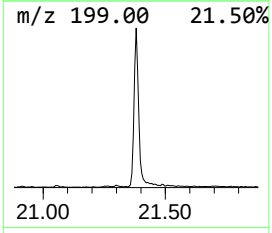
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	58
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25
5	2-Indolinone, 2TMS derivative	277	C14H23NOSi2	010416-65-6	9

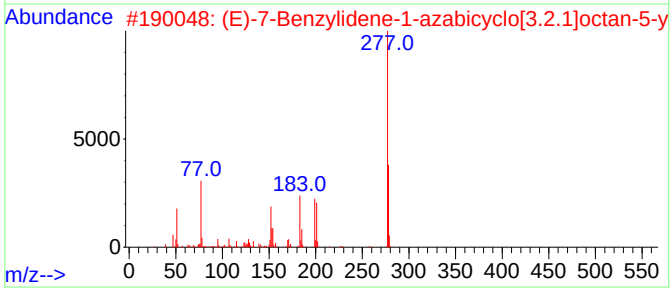


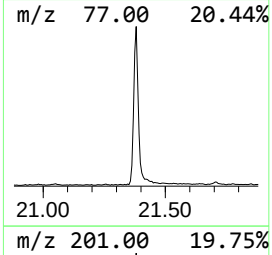


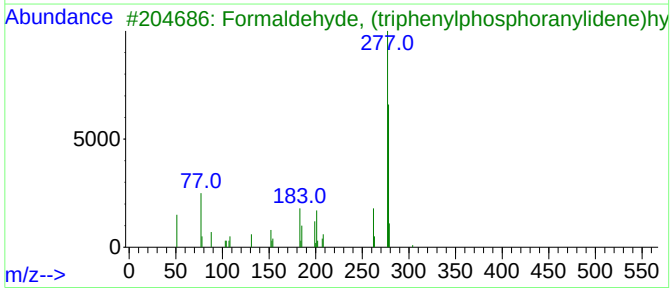


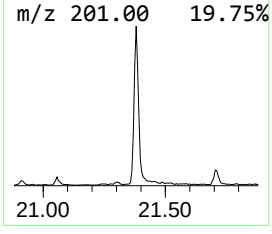












Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-...	4.875	10.0	ng	158493	1	7.740	316502	20.0
n-Hexadecanoic ...	18.063	2.7	ng	79185	4	17.163	591167	20.0
9,10-Anthracene...	18.575	6.7	ng	198515	4	17.163	591167	20.0
9-Tricosene, (Z)-	20.980	4.4	ng	197445	5	21.263	891401	20.0
Triphenylphosph...	21.380	30.7	ng	1367670	5	21.263	891401	20.0