LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP090922\
Data File : BP011668.D
Acq On : 09 Sep 2022 17:56
Operator : CG/JU
Sample : N4549-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-50D

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-BP090222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011668.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.017	3	5	13	rVB	1066341	1308325	2.13%	0.682%
2	3.093	13	18	38	rVB	12087493	15133273	24.67%	7.883%
3	5.517	423	430	442	rBV	3860016	5812814	9.47%	3.028%
4	7.116	693	702	714	rVB	2217776	3637894	5.93%	1.895%
5	7.958	837	845	853	rBV	1430825	2348885	3.83%	1.224%
6	9.128	1033	1044	1053	rBV	4804895	7829622	12.76%	4.079%
7	10.775	1316	1324	1333	rBV	1939035	3269242	5.33%	1.703%
8	13.228	1734	1741	1754	rBV	12832311	19283544	31.43%	10.045%
9	14.398	1934	1940	1950	rBV	407282	715057	1.17%	0.372%
10	14.598	1968	1974	1985	rVB	2831786	4187660	6.83%	2.181%
11	16.092	2221	2228	2249	rBV	10396326	14991574	24.44%	7.809%
12	17.357	2437	2443	2452	rVB	3399770	4860481	7.92%	2.532%
13	18.239	2588	2593	2612	rBV	2237703	3813744	6.22%	1.987%
14	19.469	2798	2802	2822	rBV	1564450	2595135	4.23%	1.352%
15	19.910	2871	2877	2882	rBV	22236601	27357580	44.59%	14.251%
16	21.433	3131	3136	3143	rBV	4313401	5664598	9.23%	2.951%
17	21.569	3152	3159	3184	rBV	35344502	61350571	100.00%	31.959%
18	21.886	3211	3213	3225	rVB	538174	828251	1.35%	0.431%
19	23.416	3469	3473	3482	rVB	581679	1051356	1.71%	0.548%
20	23.904	3550	3556	3570	rVB2	2890186	5928598	9.66%	3.088%

Sum of corrected areas: 191968204

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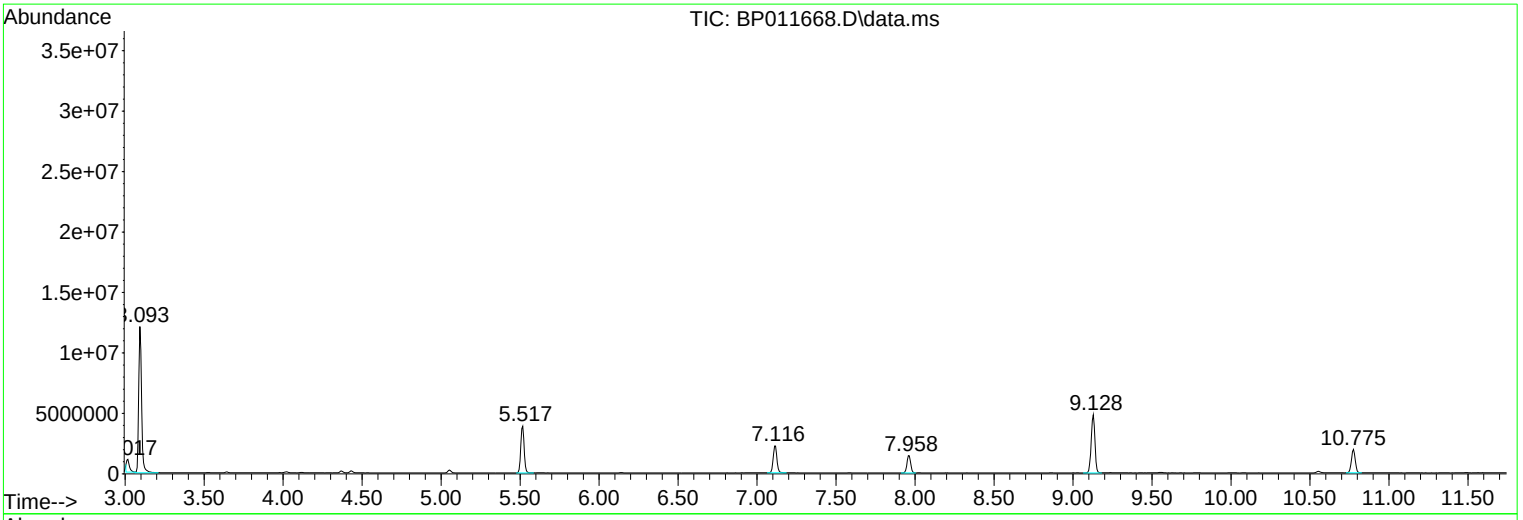
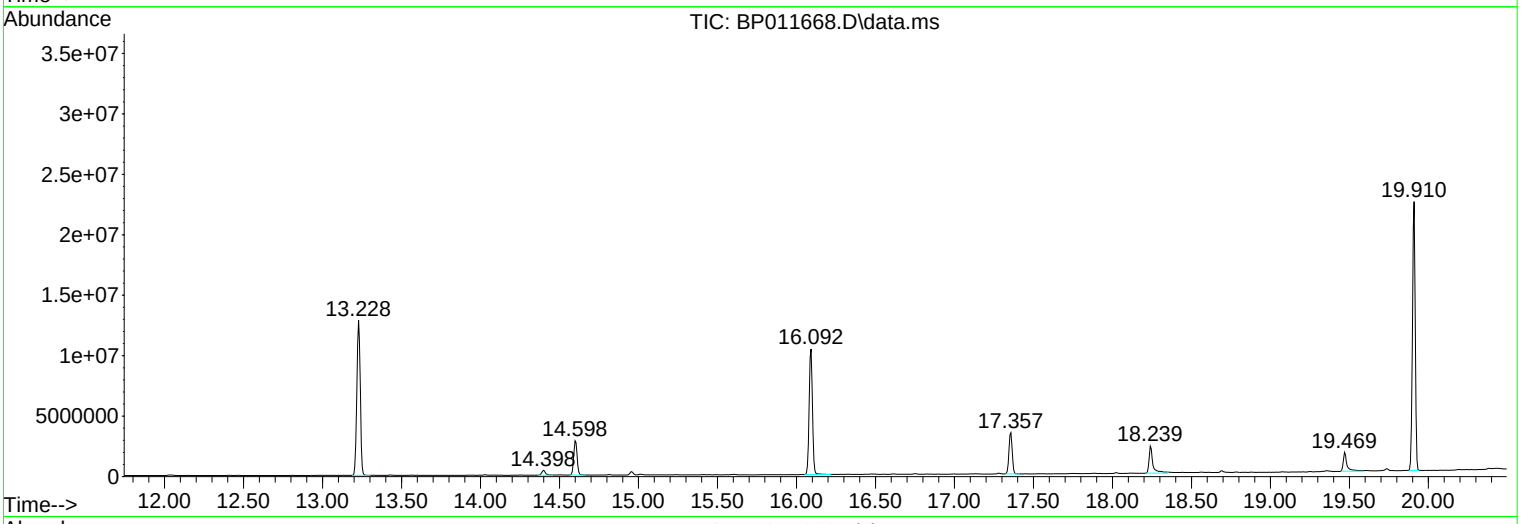
Misc :
ALS Vial : 9 Sample Multiplier: 1

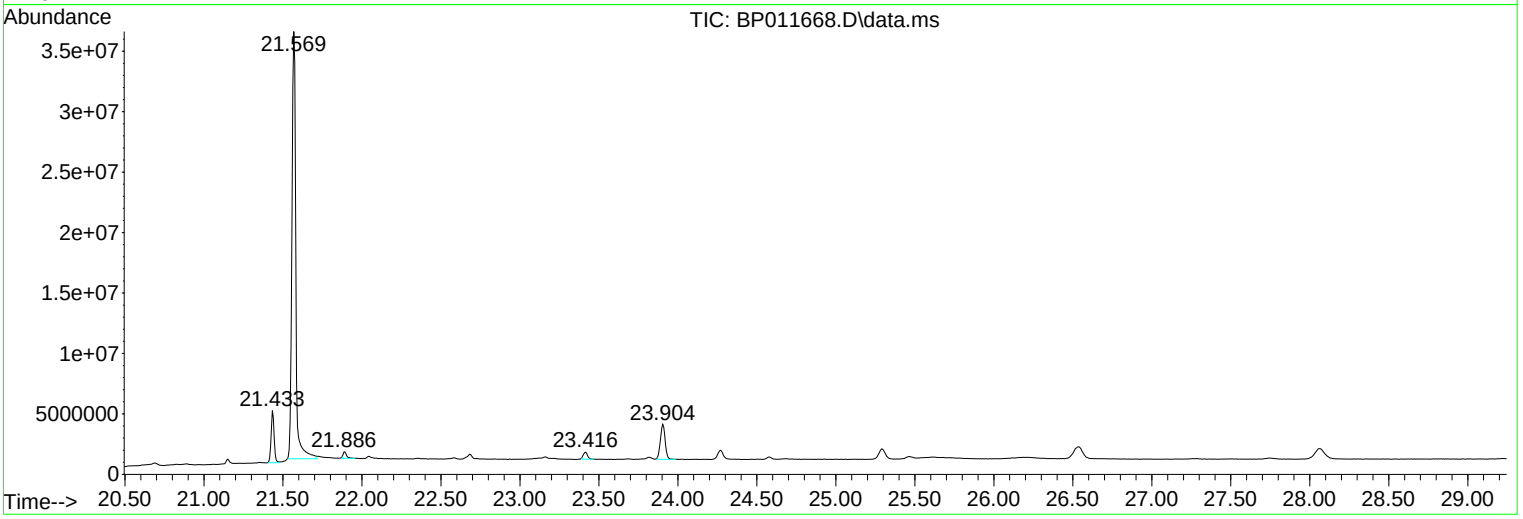
Instrument :
BNA_P
ClientSampleId :
MW-50D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.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

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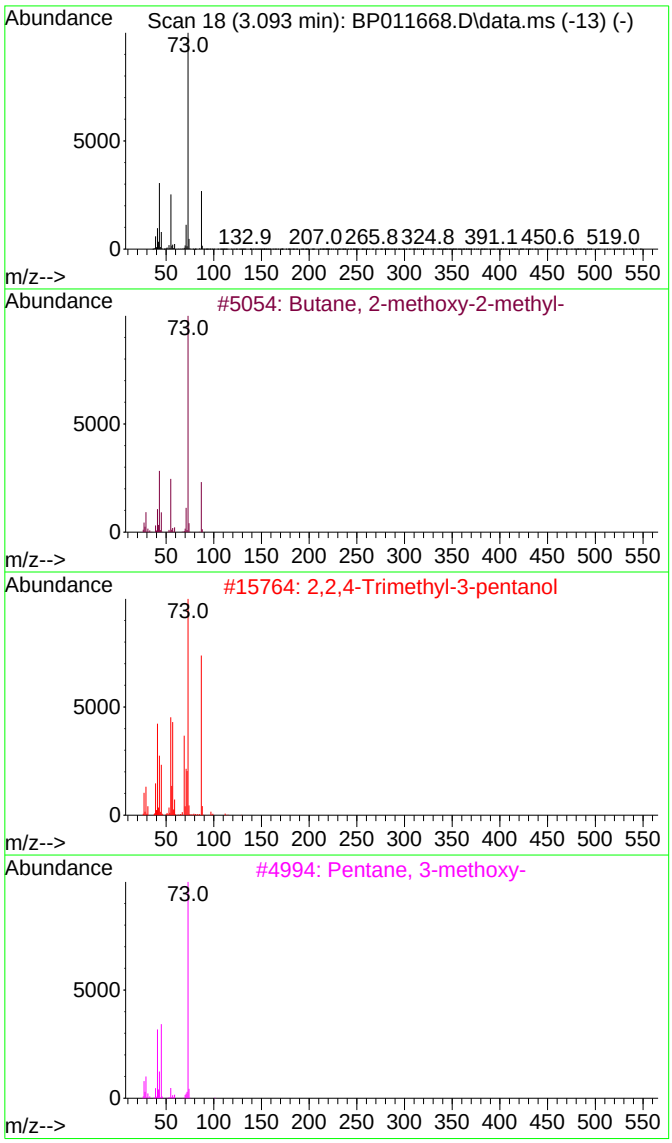
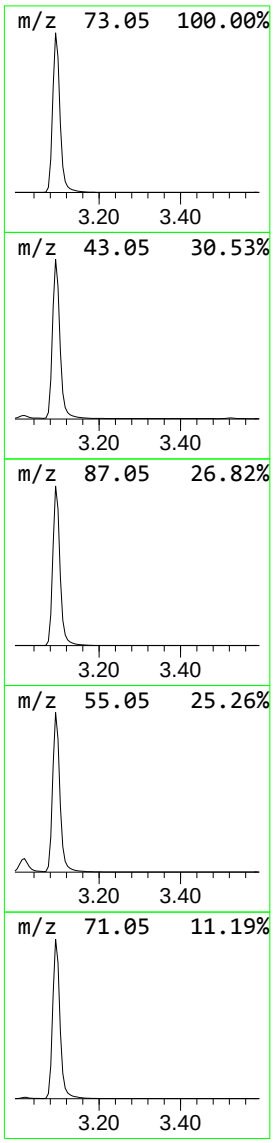
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.093	128.85 ng	15133300	1,4-Dichlorobenzene-d4	7.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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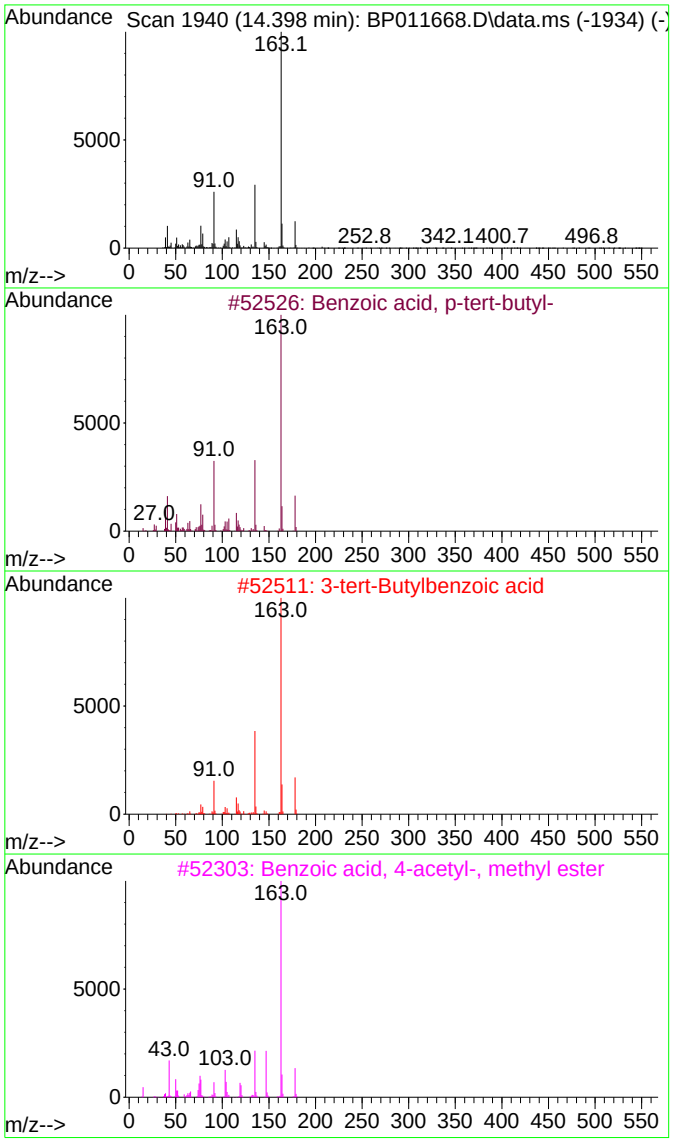
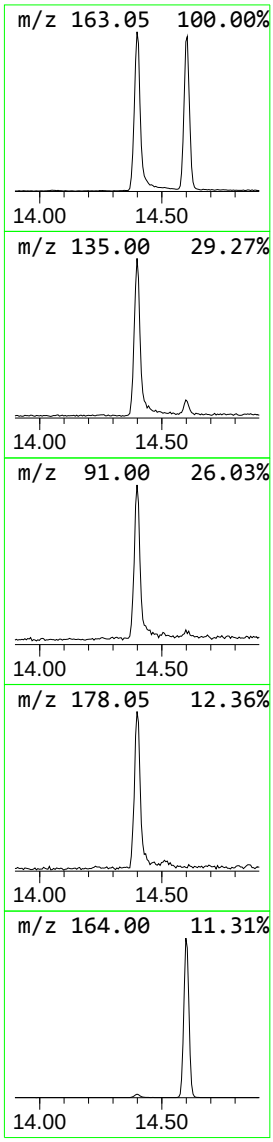
****

Peak Number 3 Benzoic acid, p-tert-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.398	3.42 ng	715057	Acenaphthene-d10	14.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	87
3	Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	72
4	1,4-Benzenedicarboxylic acid, di...	194	C10H10O4	000120-61-6	64
5	Benzonitrile, 2,4-dimethoxy-	163	C9H9NO2	004107-65-7	53





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Data File : BP011668.D
Acq On : 09 Sep 2022 17:56
Operator : CG/JU
Sample : N4549-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-50D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

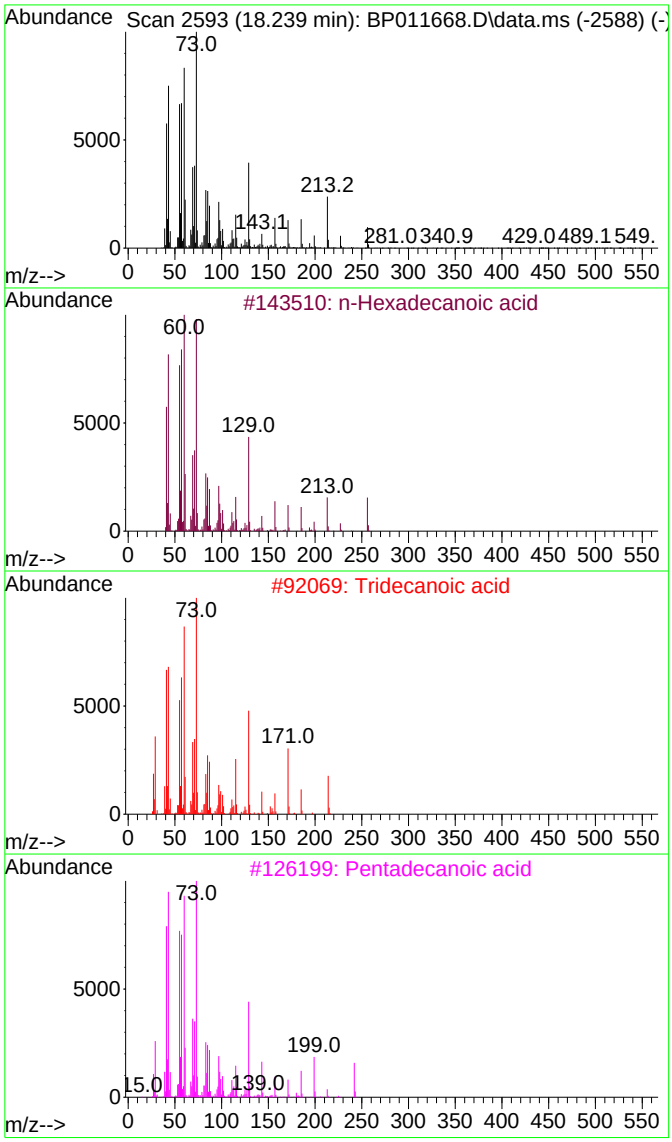
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

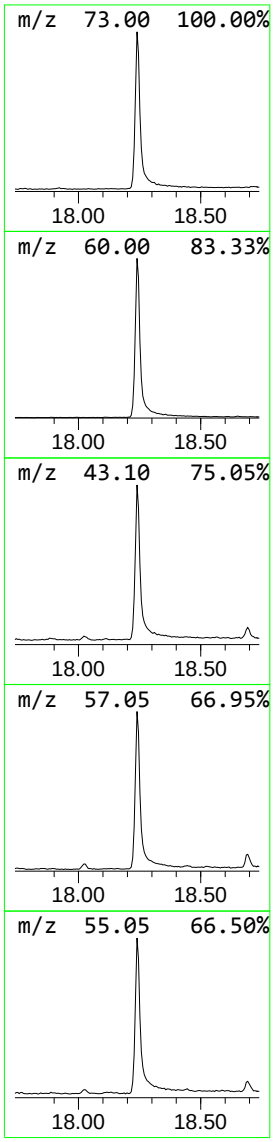
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	15.69 ng	3813740	Phenanthrene-d10	17.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Acq On : 09 Sep 2022 17:56
Operator : CG/JU
Sample : N4549-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-50D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

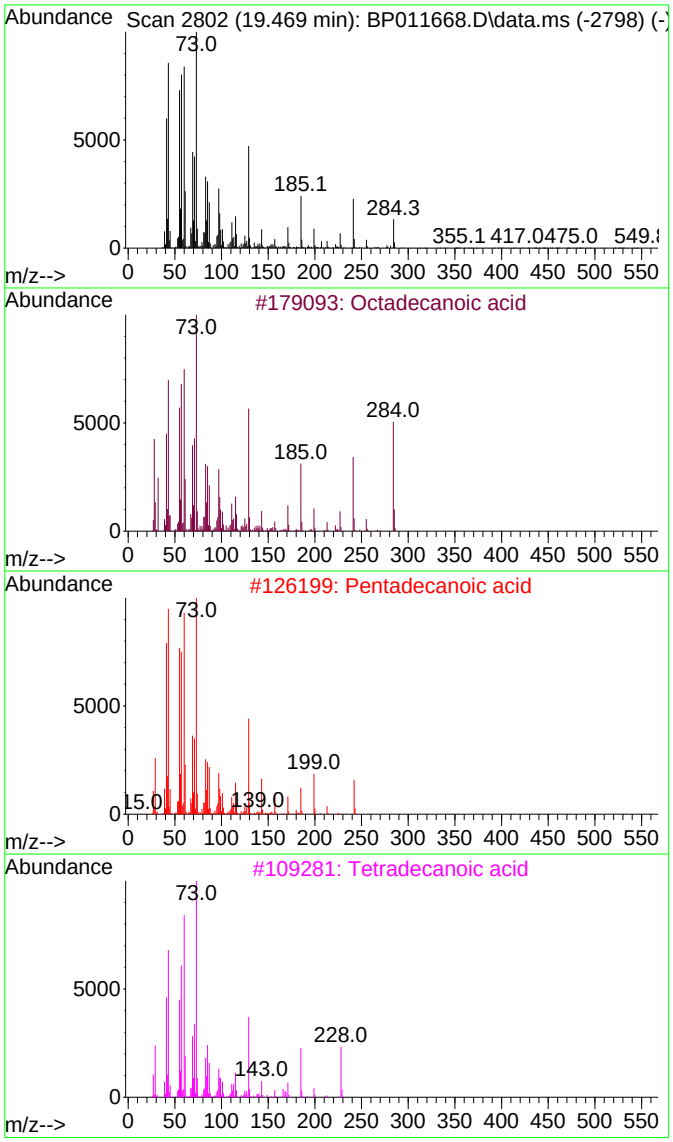
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

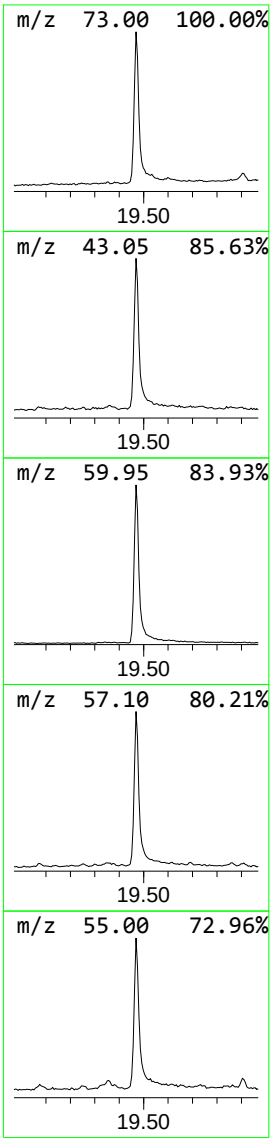
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.469	9.16 ng	2595140	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72





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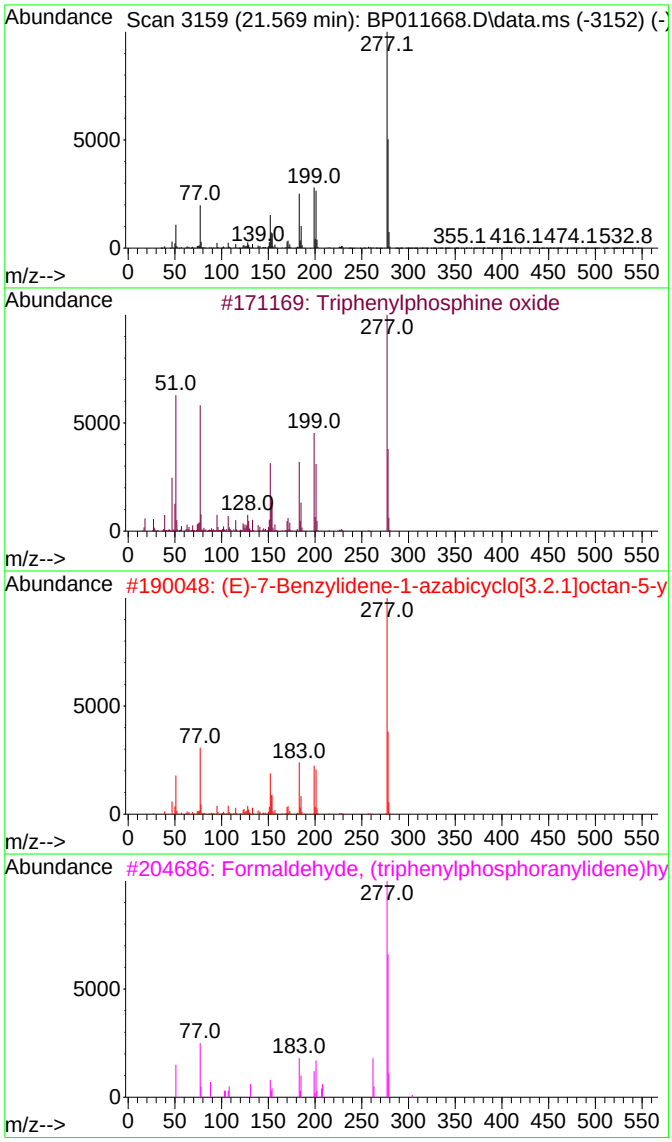
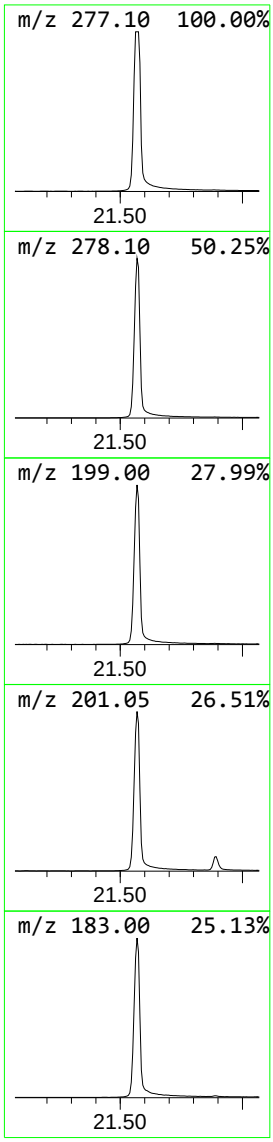
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.569	216.61 ng	61350600	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	83
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	[1,2,4]Triazolo[1,5-a]pyrimidine...	278	C15H14N6	1000350-69-0	47
5	Quinoline, 2-(2-methyl-5-nitroph...	278	C17H14N2O2	311765-54-5	37





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BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP090222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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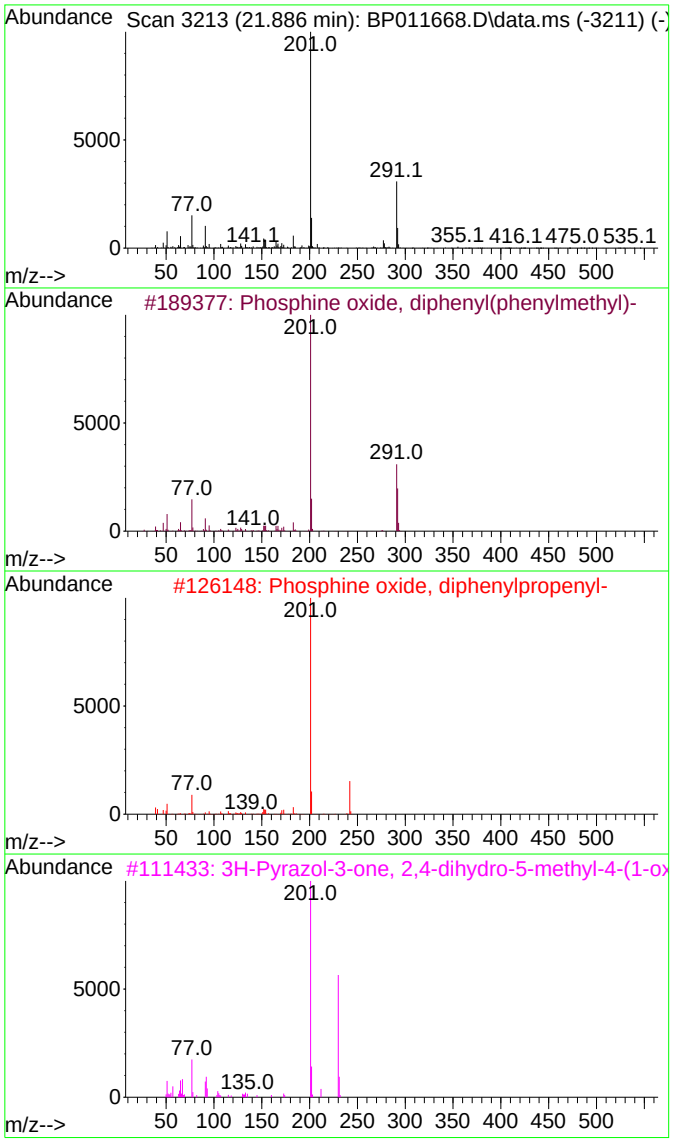
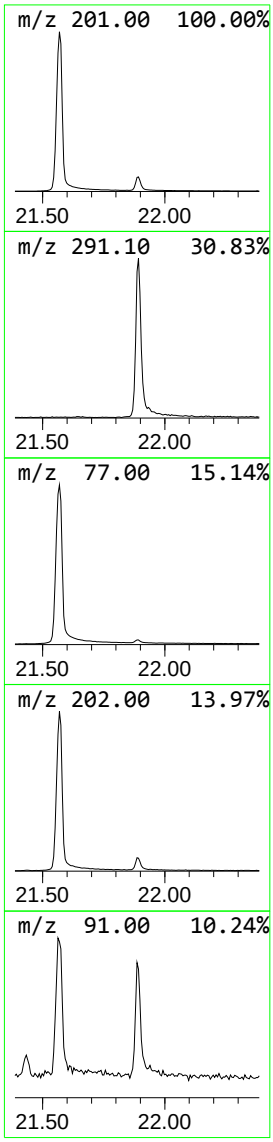
****
Peak Number 7 Phosphine oxide, diphenyl(p... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.886	2.92 ng	828251	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphine oxide, diphenyl(phenyl...	292	C19H17OP	002959-74-2	64
2	Phosphine oxide, diphenylpropenyl-	242	C15H15OP	004252-89-5	50
3	3H-Pyrazol-3-one, 2,4-dihydro-5-...	230	C13H14N2O2	031197-09-8	50
4	Phosphine, chloromethyldiphenyl-...	250	C13H12ClOP	001806-49-1	40
5	N2-Benzyl-1,3,5-triazine-2,4-dia...	201	C10H11N5	004086-63-9	40





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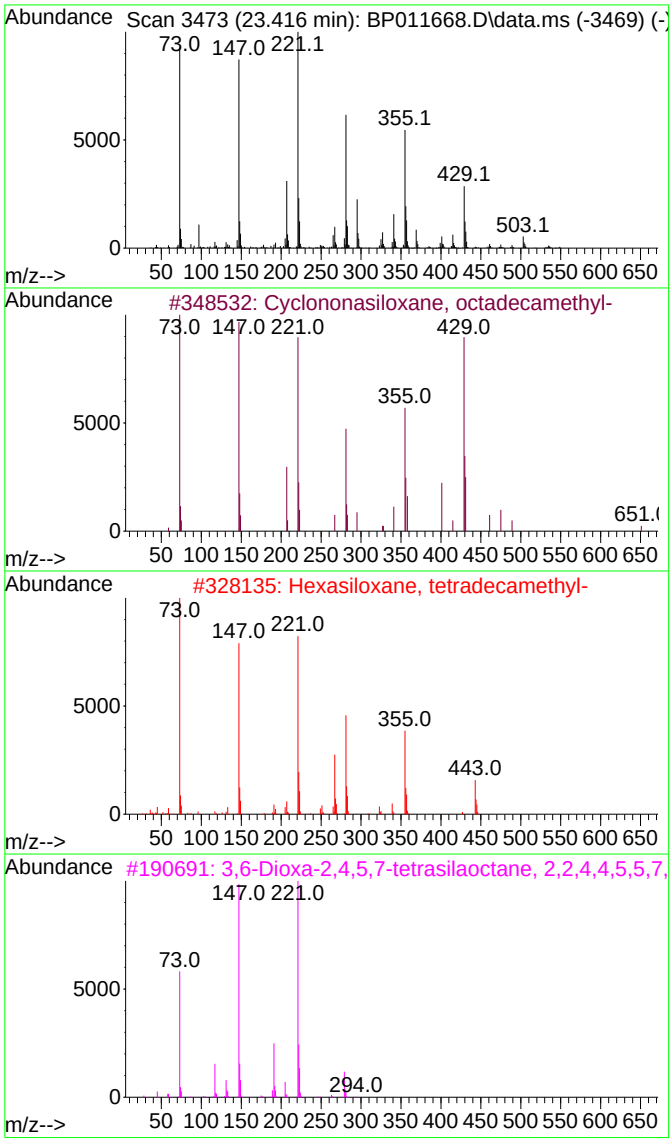
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

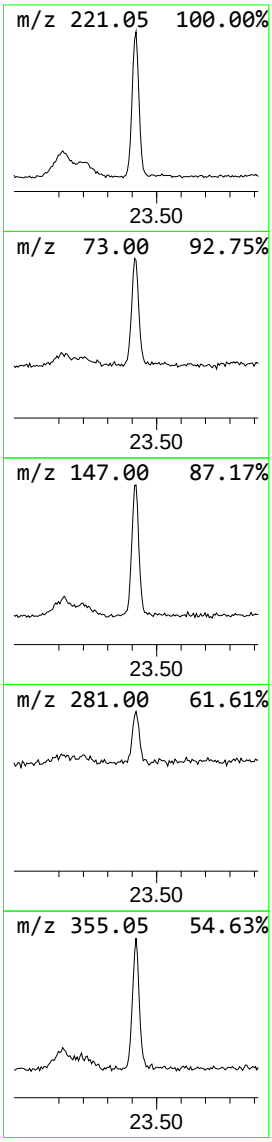
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclononasiloxane, octadeca... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.416	3.55 ng	1051360	Perylene-d12	23.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	91
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	46
4	2,5-Dihydroxybenzoic acid, 3TMS ...	370	C16H30O4Si3	003618-20-0	45
5	3,4-Dihydroxyphenylglycol, 4TMS ...	458	C20H42O4Si4	056114-62-6	25





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.093	128.8	ng	15133300	1	7.963	2348890	20.0
Benzoic acid, p...	14.398	3.4	ng	715057	3	14.598	4187660	20.0
n-Hexadecanoic ...	18.239	15.7	ng	3813740	4	17.357	4860480	20.0
Octadecanoic acid	19.469	9.2	ng	2595140	5	21.433	5664600	20.0
Triphenylphosph...	21.569	216.6	ng	61350600	5	21.433	5664600	20.0
Phosphine oxide...	21.886	2.9	ng	828251	5	21.433	5664600	20.0
Cyclononasiloxa...	23.416	3.5	ng	1051360	6	23.904	5928600	20.0