LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120821\
Data File : BP008284.D
Acq On : 08 Dec 2021 18:03
Operator : CG/JU
Sample : PB141239BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB141239BL

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-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008284.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	398	405	422	rBV	1588017	2340972	70.52%	12.651%
2	6.963	666	676	704	rBV	1354408	2261993	68.14%	12.225%
3	7.775	807	814	832	rVB	290430	468117	14.10%	2.530%
4	8.934	1002	1011	1032	rBV	812761	1434883	43.22%	7.755%
5	10.569	1281	1289	1307	rBV	292234	577802	17.40%	3.123%
6	13.045	1703	1710	1725	rBV	1818869	2750438	82.85%	14.864%
7	14.428	1938	1945	1956	rBV	424935	664790	20.03%	3.593%
8	15.928	2193	2200	2222	rBV	1174764	1856351	55.92%	10.032%
9	17.192	2409	2415	2433	rBV	428963	699521	21.07%	3.780%
10	19.475	2799	2803	2809	rBV	94793	99601	3.00%	0.538%
11	19.763	2847	2852	2861	rBV	2623398	3319787	100.00%	17.941%
12	20.498	2973	2977	2983	rBV	77388	96506	2.91%	0.522%
13	21.086	3073	3077	3084	rBV	72969	124646	3.75%	0.674%
14	21.304	3109	3114	3121	rBV	548405	777408	23.42%	4.201%
15	21.416	3130	3133	3138	rBV	129789	191901	5.78%	1.037%
16	23.692	3514	3520	3531	rVB	395893	838953	25.27%	4.534%

Sum of corrected areas: 18503669

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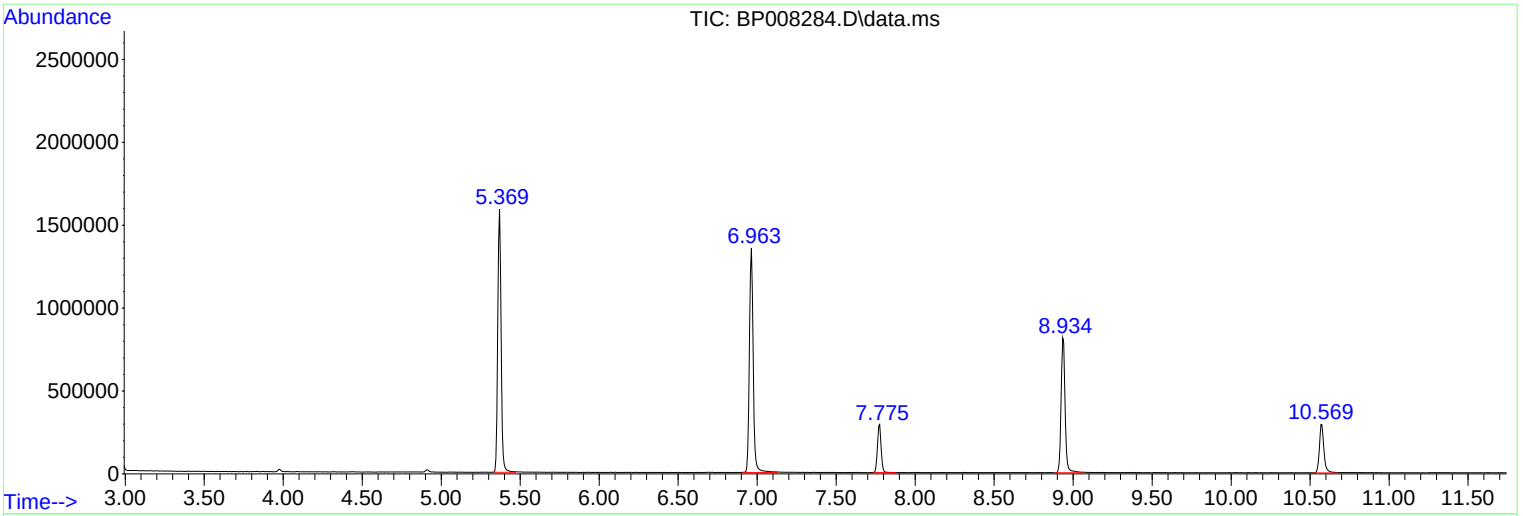
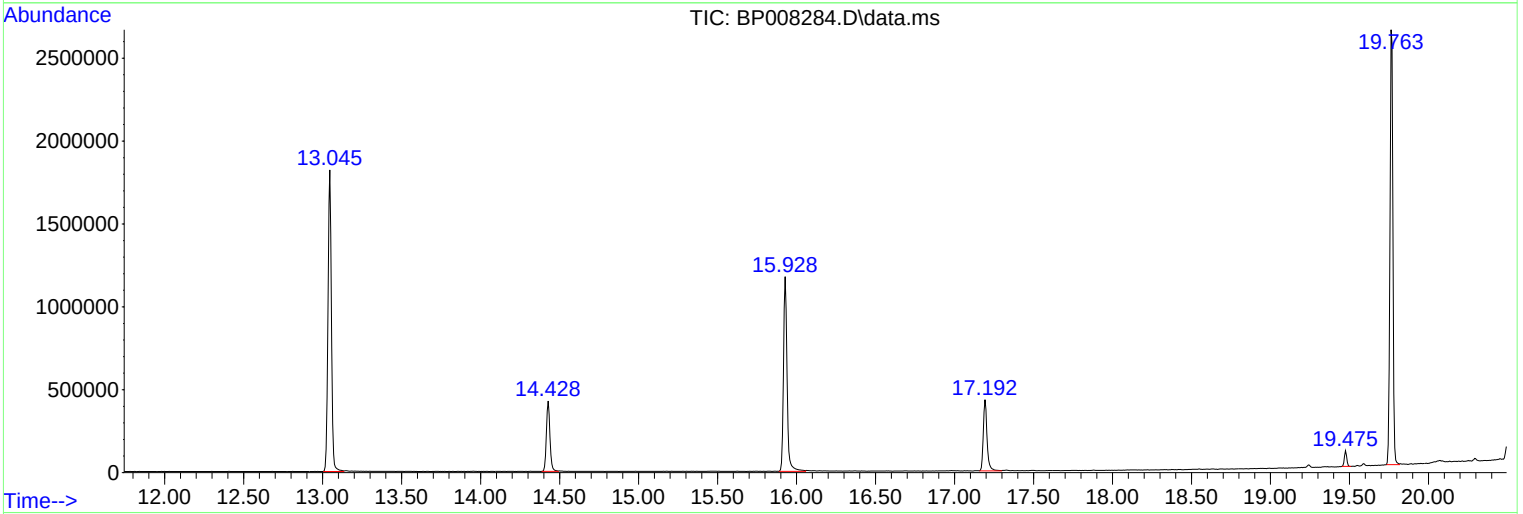
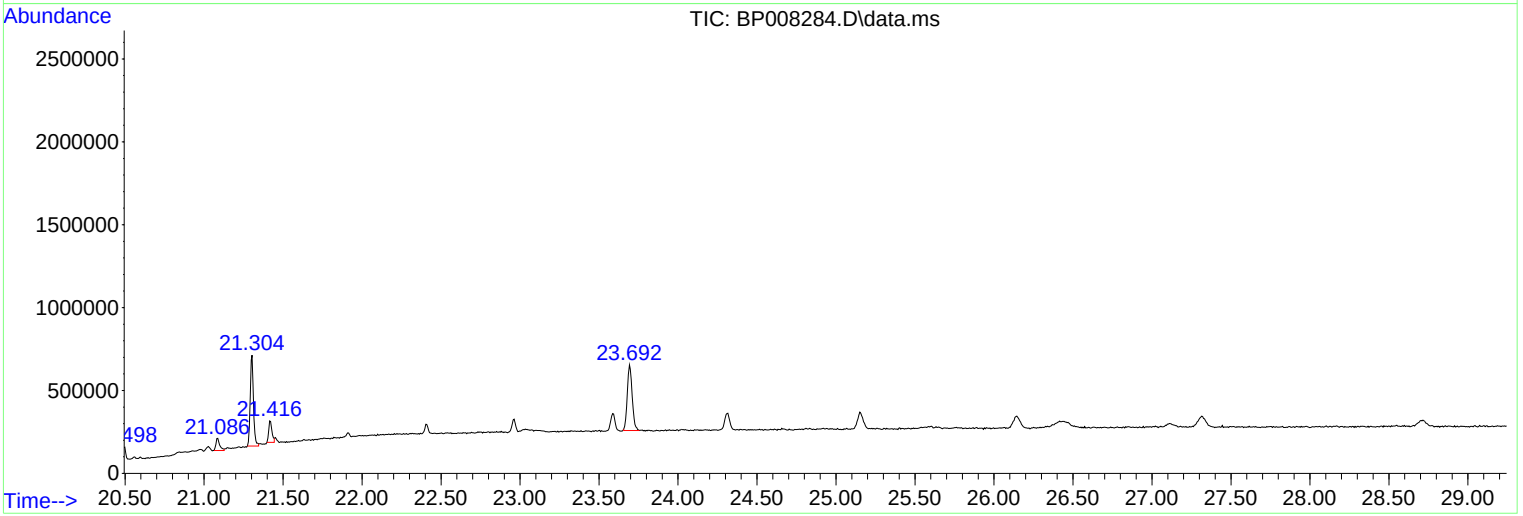
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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ClientSampleId :
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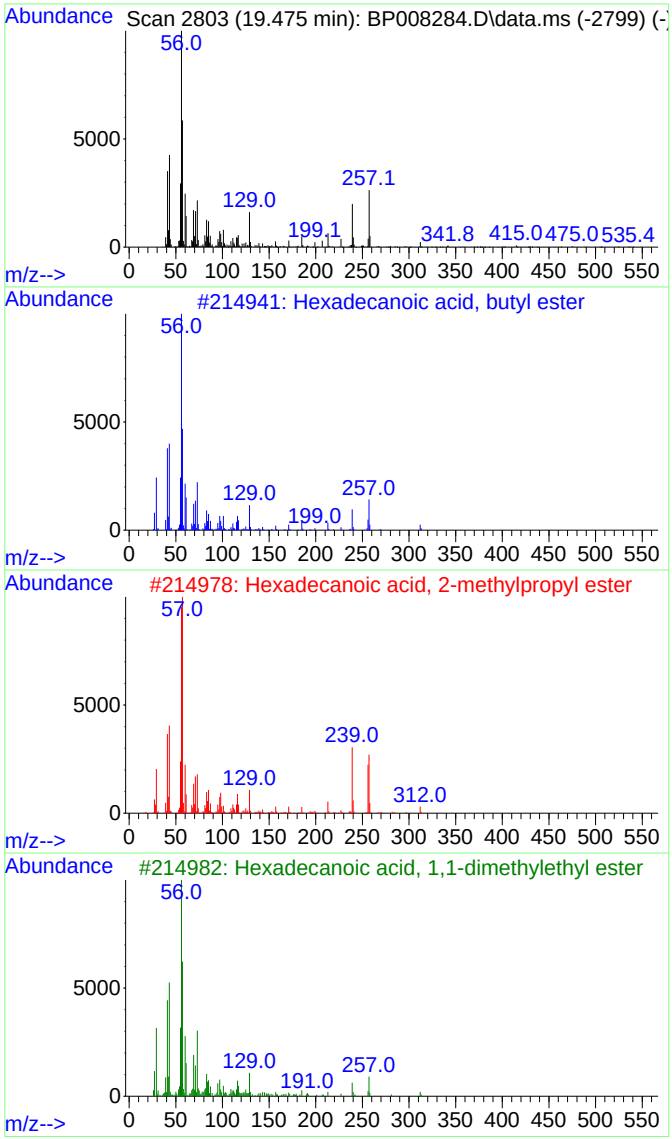
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

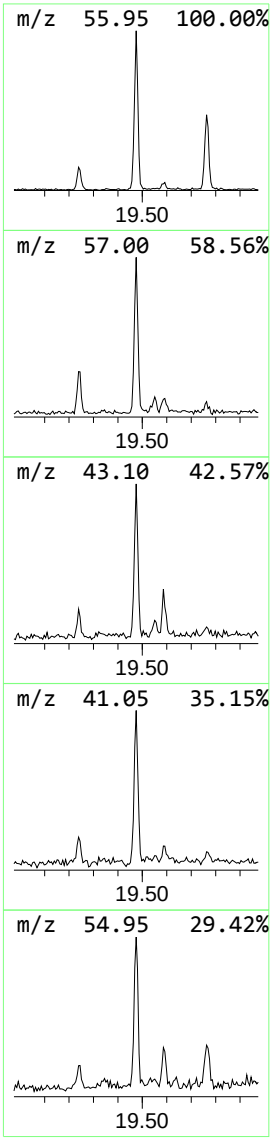
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.474	2.56 ng	99601	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	81
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	55
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	30
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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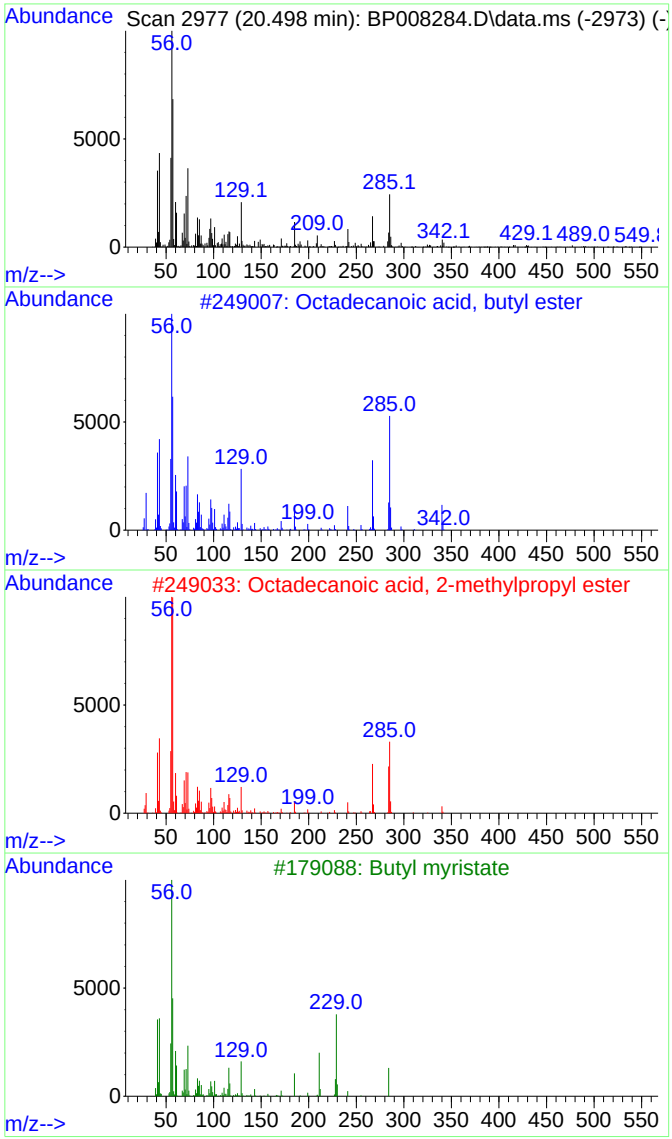
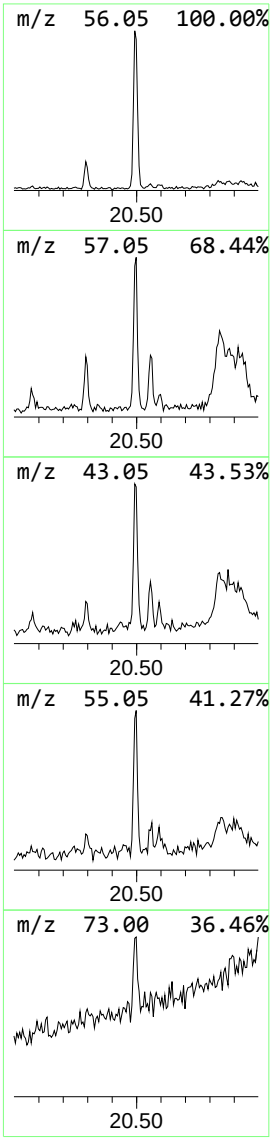
Peak Number 2 Octadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.498	2.48 ng	96506	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	98
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	87
3	Butyl myristate	284	C18H36O2	000110-36-1	59
4	Piperidin-4-carboxylic acid	129	C6H11NO2	000498-94-2	43
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38





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Data File : BP008284.D
Acq On : 08 Dec 2021 18:03
Operator : CG/JU
Sample : PB141239BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB141239BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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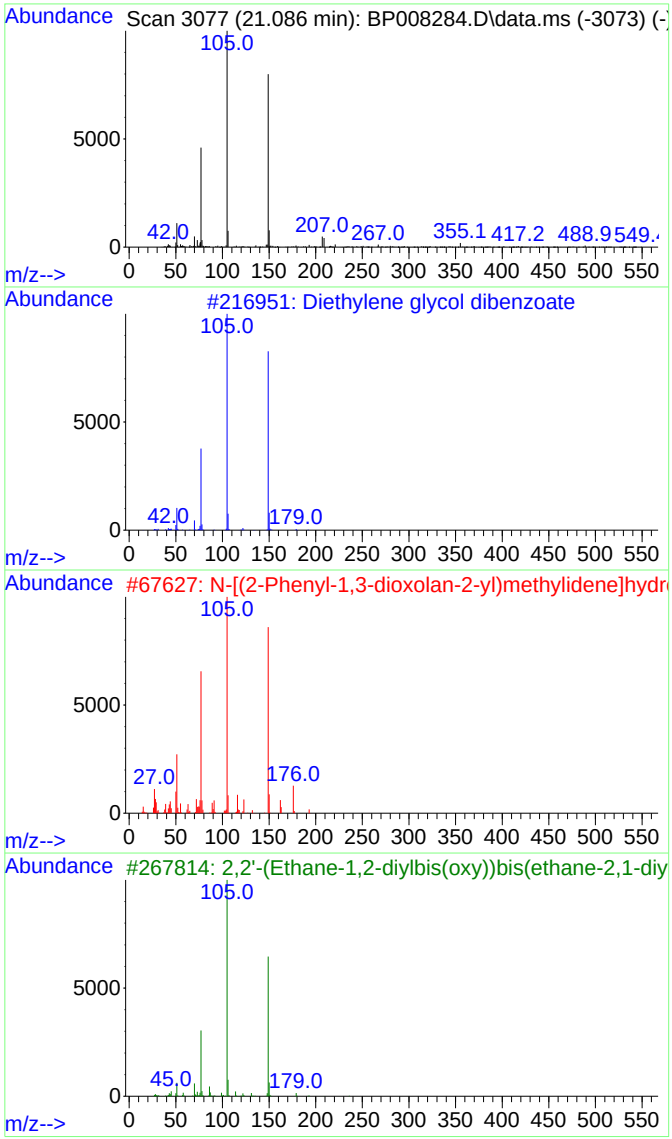
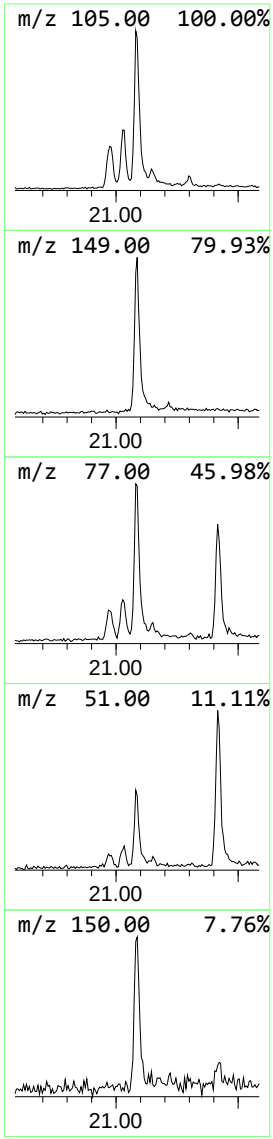
Peak Number 3 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.086	3.21 ng	124646	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	N-[(2-Phenyl-1,3-dioxolan-2-yl)m...	193	C10H11NO3	1000411-48-9	72
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	53
4	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50
5	Benzoic acid, (2-methyl-3-nitrop...	271	C15H13NO4	1000367-95-0	43





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Sample : PB141239BL
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ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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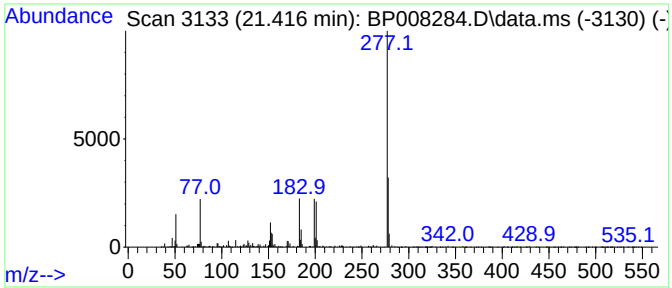
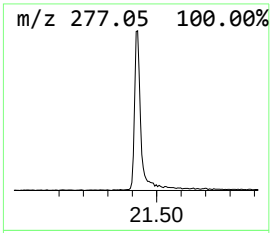
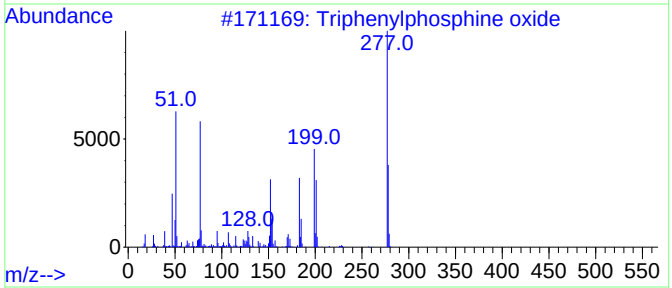
Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

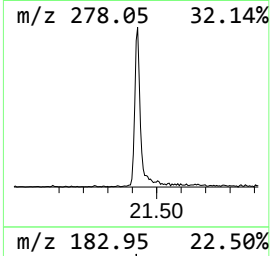
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	4.94 ng	191901	Chrysene-d12	21.304

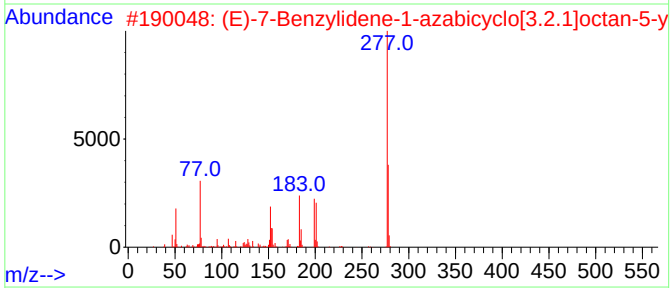
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	64
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	40
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	32

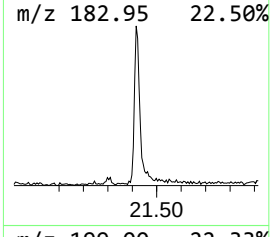


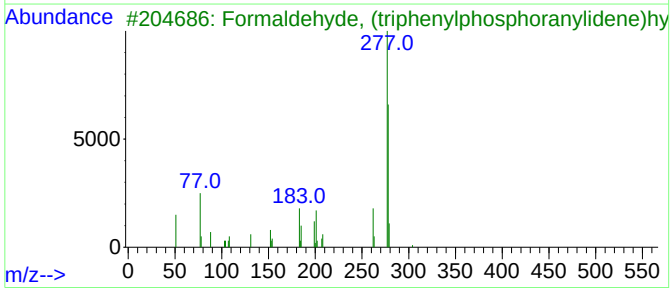


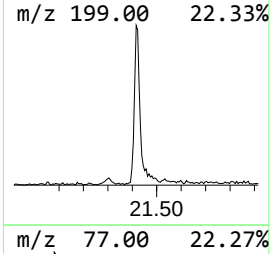


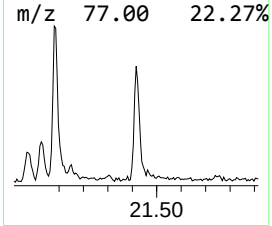












Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexadecanoic ac...	19.474	2.6	ng	99601	5	21.304	777408	20.0
Octadecanoic ac...	20.498	2.5	ng	96506	5	21.304	777408	20.0
Diethylene glyc...	21.086	3.2	ng	124646	5	21.304	777408	20.0
Triphenylphosph...	21.416	4.9	ng	191901	5	21.304	777408	20.0