LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
Data File : BP008163.D
Acq On : 30 Nov 2021 17:50
Operator : CG/JU
Sample : M4849-01 10X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-1-112921

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: BP008163.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	325	330	338	rVB	26650	39452	2.44%	0.758%
2	5.393	403	409	418	rBV	229983	346231	21.40%	6.651%
3	6.981	671	679	695	rBV	210862	367948	22.74%	7.068%
4	7.799	811	818	826	rBV	60642	101146	6.25%	1.943%
5	8.963	1008	1016	1025	rBV	125638	225699	13.95%	4.336%
6	10.599	1287	1294	1301	rBV	76451	136122	8.41%	2.615%
7	13.069	1708	1714	1725	rBV	338604	524159	32.40%	10.069%
8	14.316	1919	1926	1930	rBV3	14365	37523	2.32%	0.721%
9	14.445	1942	1948	1955	rBV	106732	162734	10.06%	3.126%
10	15.945	2197	2203	2217	rBV	195551	341411	21.10%	6.558%
11	17.139	2401	2406	2412	rBV9	12906	21623	1.34%	0.415%
12	17.210	2412	2418	2423	rBV	122977	188915	11.68%	3.629%
13	17.886	2530	2533	2537	rVB2	16947	21401	1.32%	0.411%
14	18.110	2567	2571	2574	rBV5	11007	16730	1.03%	0.321%
15	19.227	2757	2761	2767	rBV	36485	56205	3.47%	1.080%
16	19.575	2817	2820	2825	rBV	38179	51861	3.21%	0.996%
17	19.774	2850	2854	2859	rBV	484538	562451	34.77%	10.804%
18	21.086	3073	3077	3083	rBV	188665	244913	15.14%	4.705%
19	21.304	3111	3114	3119	rVB	105901	141402	8.74%	2.716%
20	21.421	3130	3134	3145	rBV	1122641	1617814	100.00%	31.078%

Sum of corrected areas: 5205740

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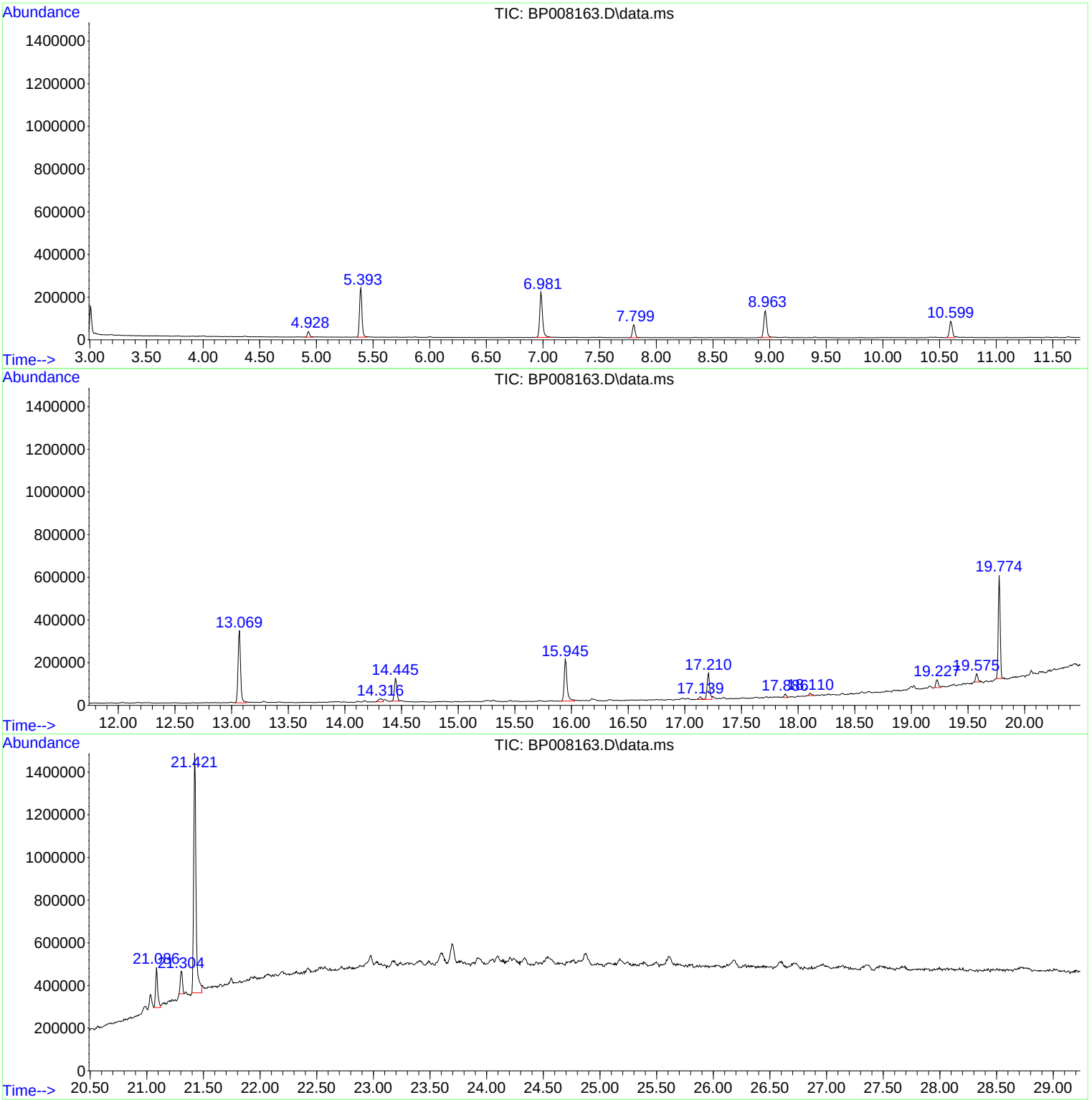
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HD-1-112921

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP113021\
Data File : BP008163.D
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TIC Library : C:\Database\NIST20.L
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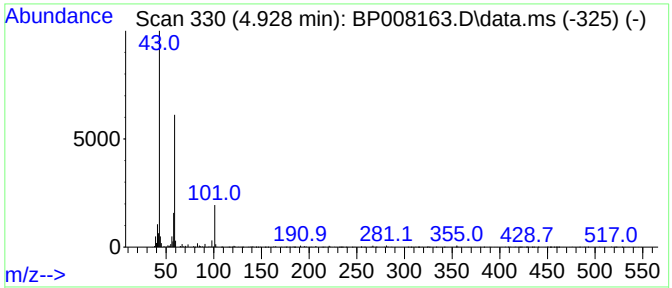
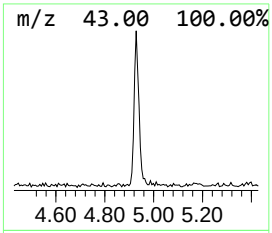
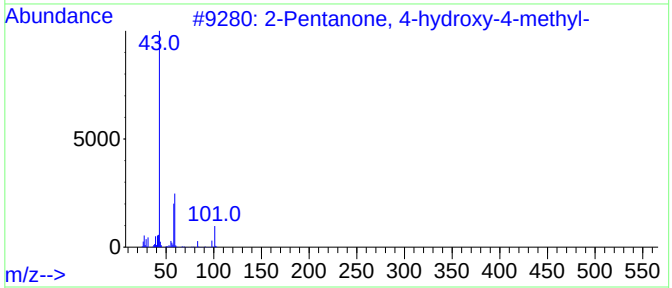
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

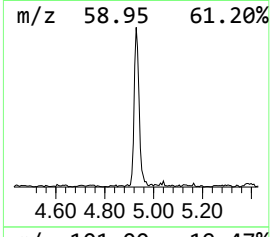
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	7.80 ng	39452	1,4-Dichlorobenzene-d4	7.805

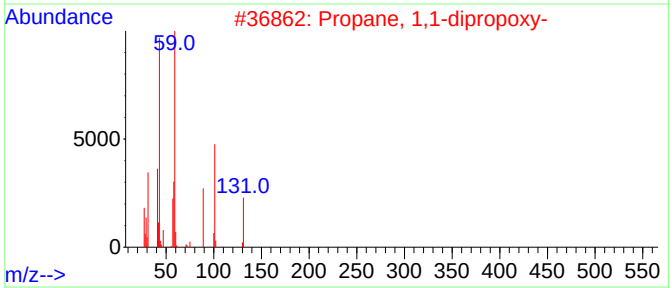
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
3	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	38
4	3-Octanol	130	C8H18O	000589-98-0	33
5	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28

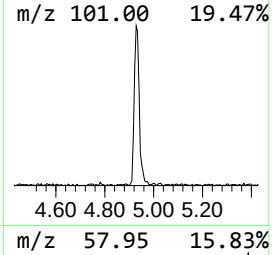


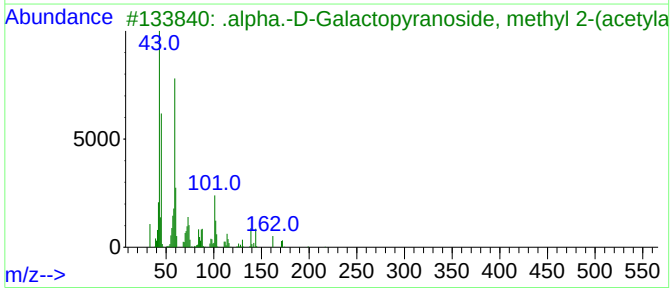


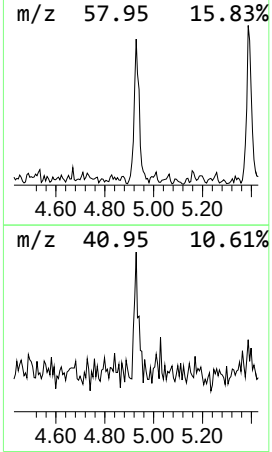












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Misc :
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Instrument :
BNA_P
ClientSampleId :
HD-1-112921

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

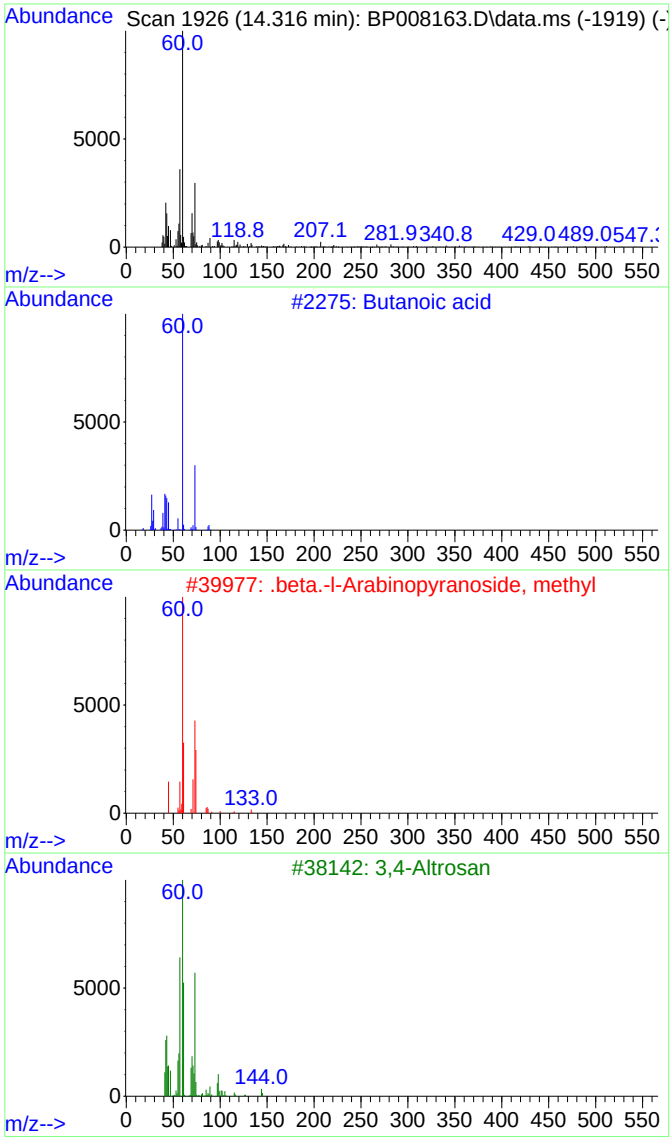
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

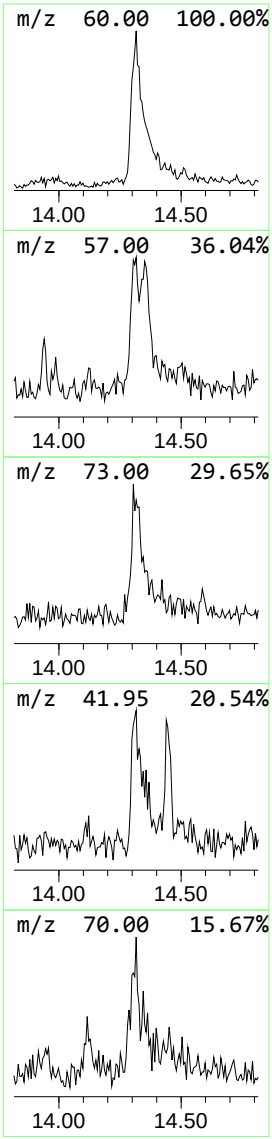
****

Peak Number 2 Butanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.316	4.61 ng	37523	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	59
2	.beta.-l-Arabinopyranoside, methyl	164	C6H12O5	001825-00-9	50
3	3,4-Altrosan	162	C6H10O5	1000129-76-4	47
4	Pentanoic acid	102	C5H10O2	000109-52-4	45
5	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	45





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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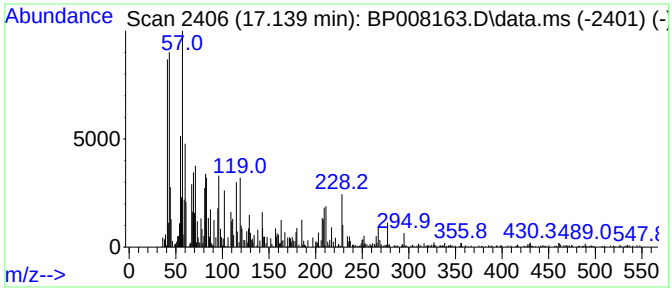
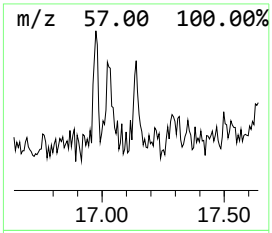
****

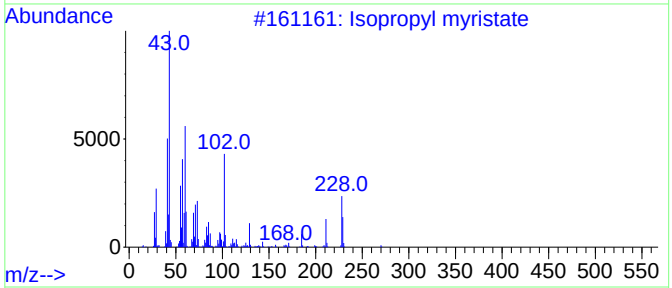
Peak Number 3 unknown17.139 Concentration Rank 5

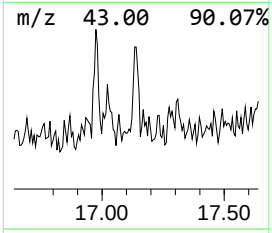
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.139	2.29 ng	21623	Phenanthrene-d10	17.210

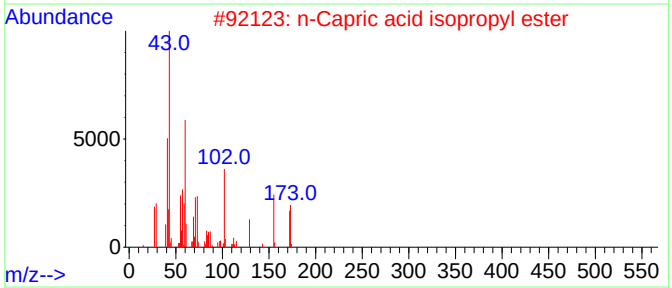
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl myristate	270	C17H34O2	000110-27-0	27
2	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	22
3	Butanoic acid, 3-methyl-, 1-meth...	144	C8H16O2	032665-23-9	12
4	o-Acetyl-L-serine	147	C5H9NO4	005147-00-2	12
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	10

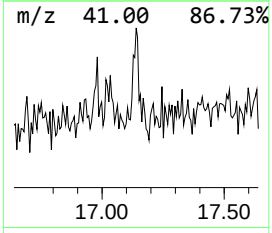


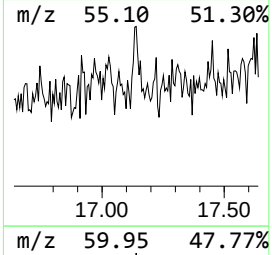


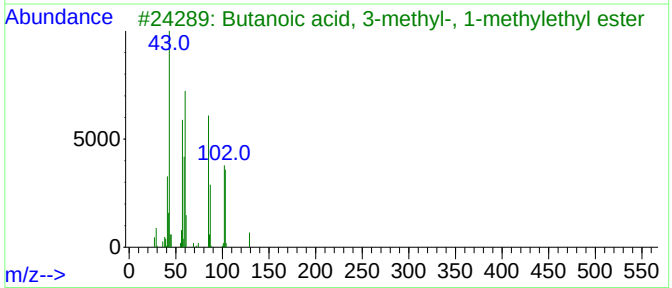


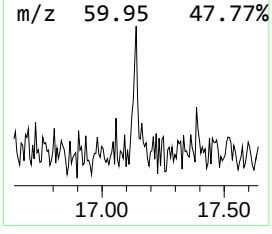












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

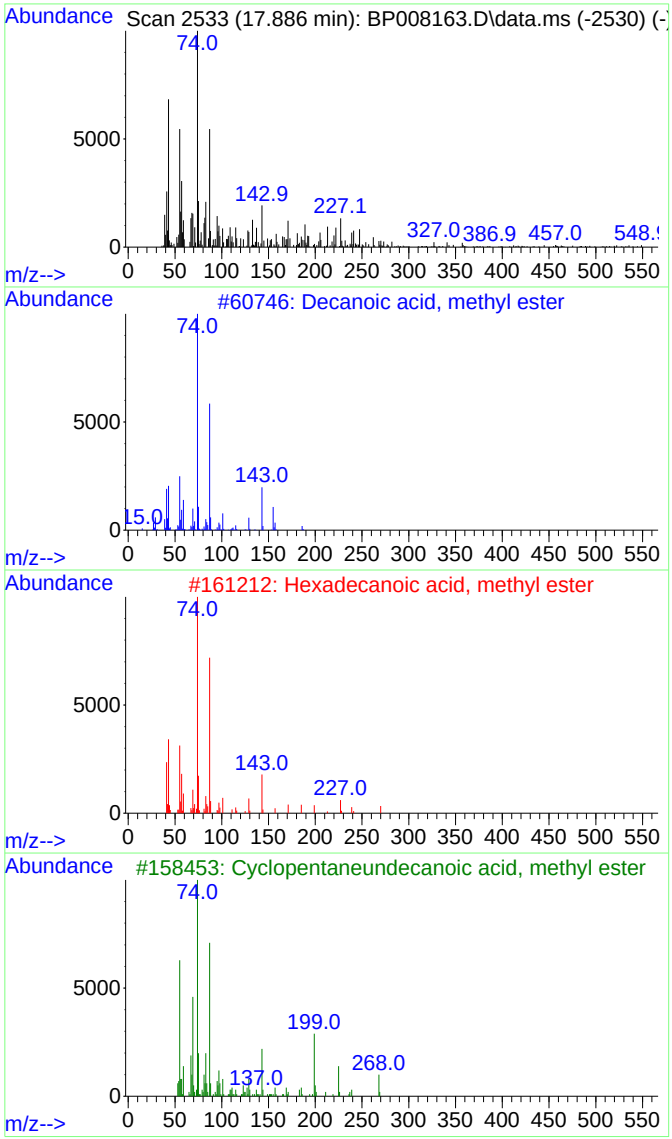
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

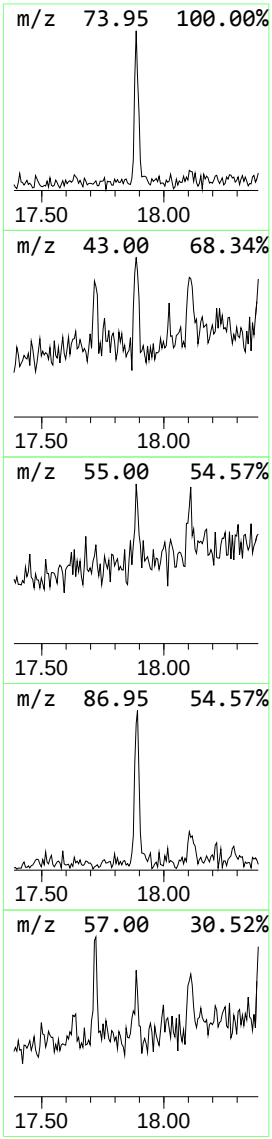
****

Peak Number 4 Decanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.886	2.27 ng	21401	Phenanthrene-d10	17.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87
3	Cyclopentaneundecanoic acid, met...	268	C17H32O2	025779-85-5	83
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	81
5	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	81





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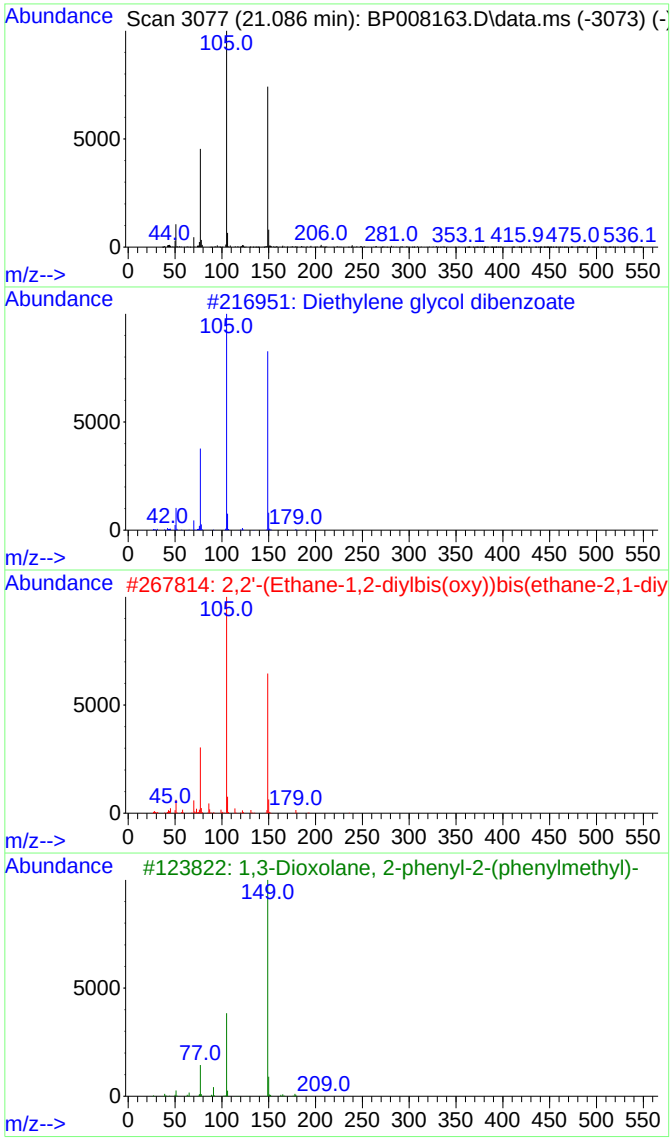
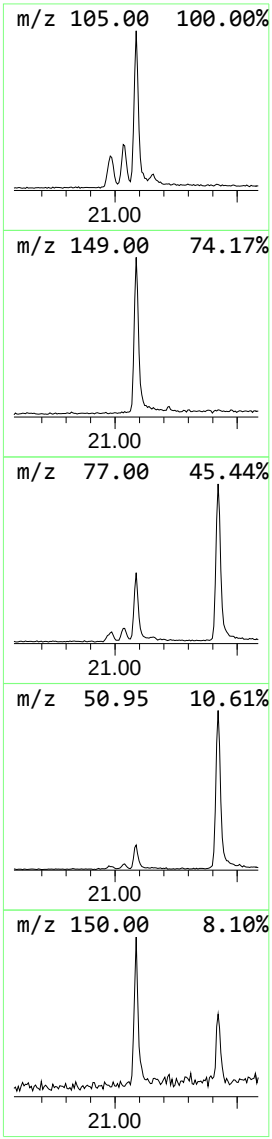
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.086	34.64 ng	244913	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
3	1,3-Dioxolane, 2-phenyl-2-(pheny...	240	C16H16O2	004362-19-0	74
4	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
5	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64





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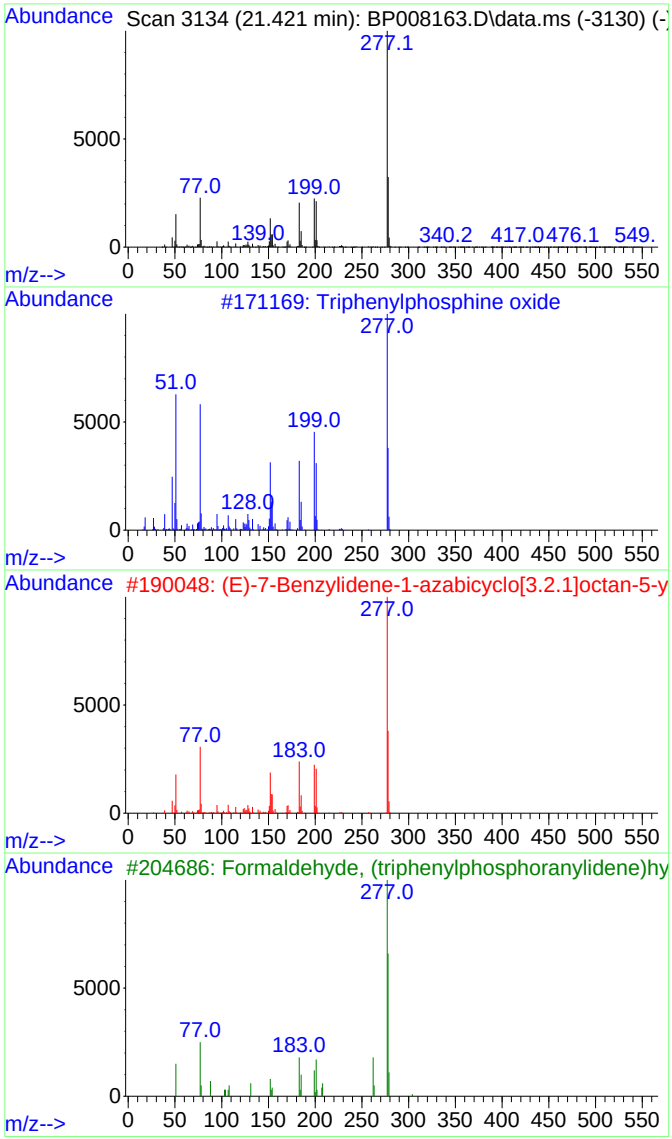
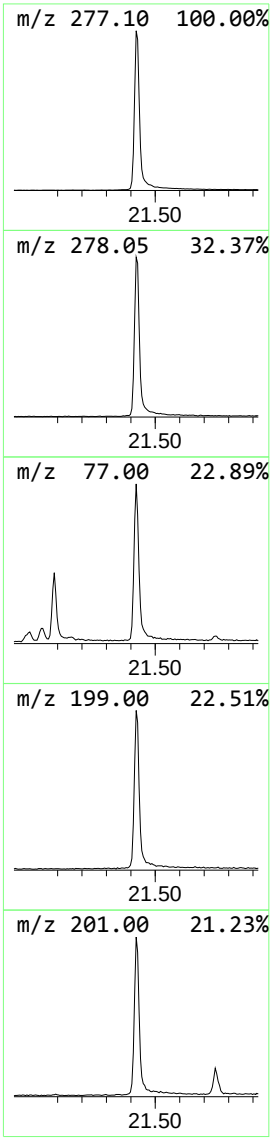
****

Peak Number 6 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.422	228.82 ng	1617810	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	70
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32
5	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	25





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
2-Pentanone, 4-...	4.928	7.8	ng	39452	1	7.805	101146	20.0
Butanoic acid	14.316	4.6	ng	37523	3	14.445	162734	20.0
unknown17.139	17.139	2.3	ng	21623	4	17.210	188915	20.0
Decanoic acid, ...	17.886	2.3	ng	21401	4	17.210	188915	20.0
Diethylene glyc...	21.086	34.6	ng	244913	5	21.304	141402	20.0
Triphenylphosph...	21.422	228.8	ng	1617810	5	21.304	141402	20.0