LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
Data File : BP009431.D
Acq On : 16 Mar 2022 20:01
Operator : CG/JU
Sample : N1956-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TPK-3

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-BP030522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009431.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.052	7	11	18	rVB	387000	528594	3.73%	0.600%
2	3.611	96	106	133	rBV	4303870	8759390	61.81%	9.950%
3	3.811	135	140	155	rVB	192897	408008	2.88%	0.463%
4	4.946	327	333	344	rBV	541417	885726	6.25%	1.006%
5	5.422	407	414	430	rBV	3476089	5970842	42.13%	6.783%
6	7.011	671	684	695	rBV	4499541	8055905	56.84%	9.151%
7	7.111	695	701	713	rVB	260608	499434	3.52%	0.567%
8	7.810	806	820	828	rBV	1360751	2378112	16.78%	2.701%
9	8.963	1008	1016	1028	rBV	2541171	4602413	32.48%	5.228%
10	10.604	1285	1295	1309	rBV	1853146	3566434	25.17%	4.051%
11	13.075	1707	1715	1734	rBV	7688445	12423097	87.66%	14.112%
12	14.363	1931	1934	1939	rVB	109781	159814	1.13%	0.182%
13	14.451	1942	1949	1960	rVV	3046244	4937864	34.84%	5.609%
14	15.734	2163	2167	2172	rVB2	99424	164316	1.16%	0.187%
15	15.951	2198	2204	2214	rBV	3114850	4800842	33.88%	5.453%
16	16.187	2240	2244	2246	rBV	177366	246179	1.74%	0.280%
17	17.216	2413	2419	2425	rBV	3512214	5620929	39.66%	6.385%
18	18.128	2570	2574	2581	rBV3	344508	618433	4.36%	0.703%
19	19.233	2760	2762	2766	rBV	352087	413516	2.92%	0.470%
20	19.792	2852	2857	2863	rBV	11510825	14171847	100.00%	16.098%
21	21.327	3114	3118	3122	rVB	3508020	4607824	32.51%	5.234%
22	23.739	3525	3528	3535	rVB2	2305521	4213374	29.73%	4.786%

Sum of corrected areas: 88032893

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
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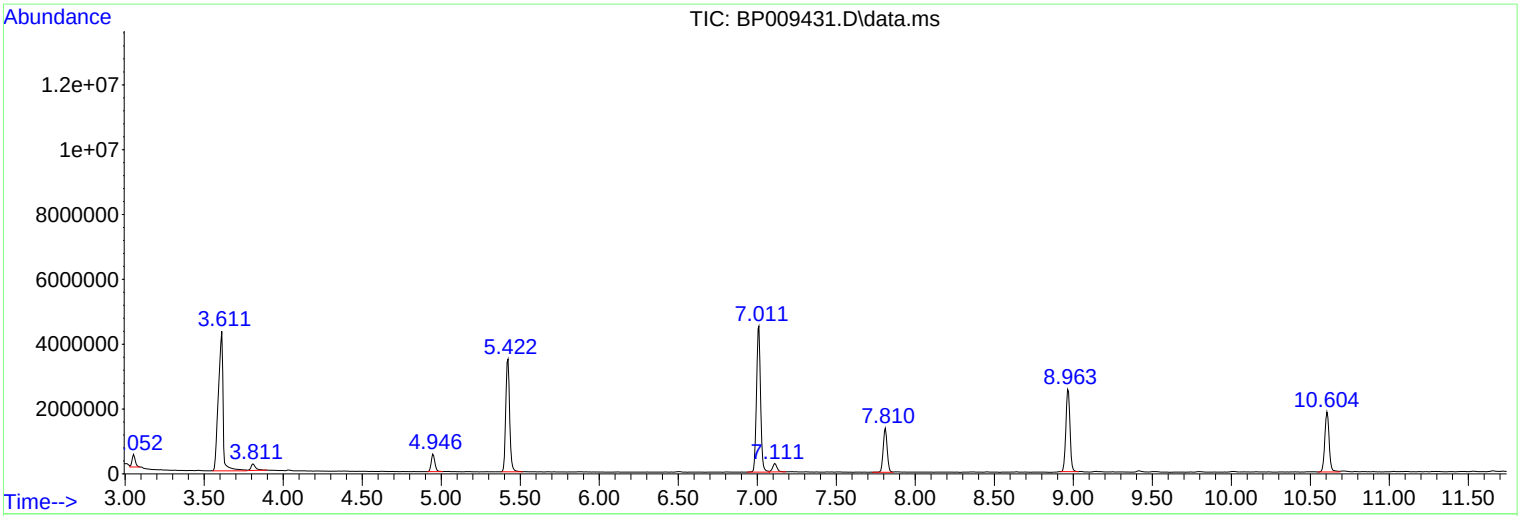
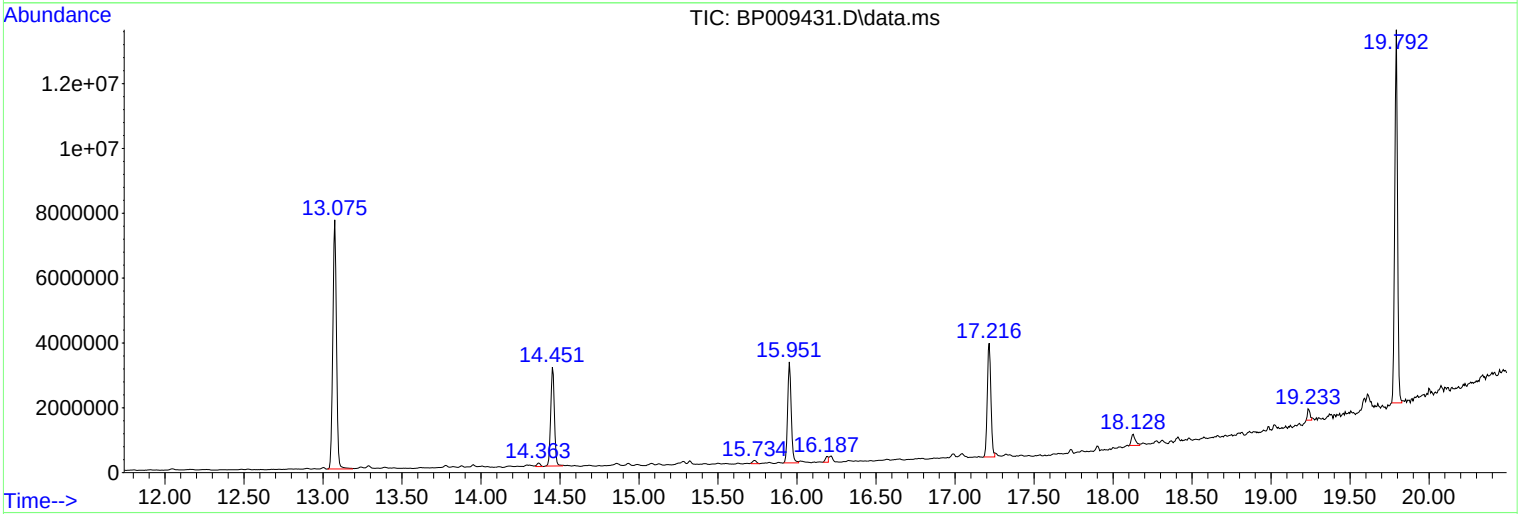
Sample : N1956-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

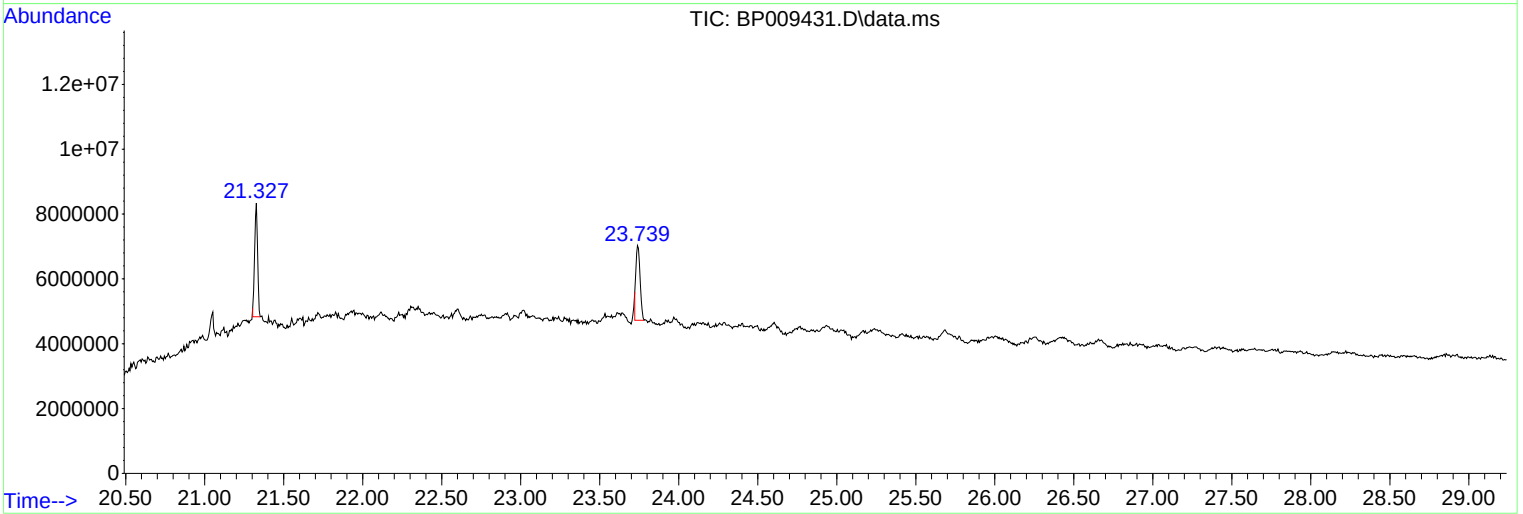
Instrument :
BNA_P
ClientSampleId :
TPK-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.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\BP031622\
Data File : BP009431.D
Acq On : 16 Mar 2022 20:01
Operator : CG/JU
Sample : N1956-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TPK-3

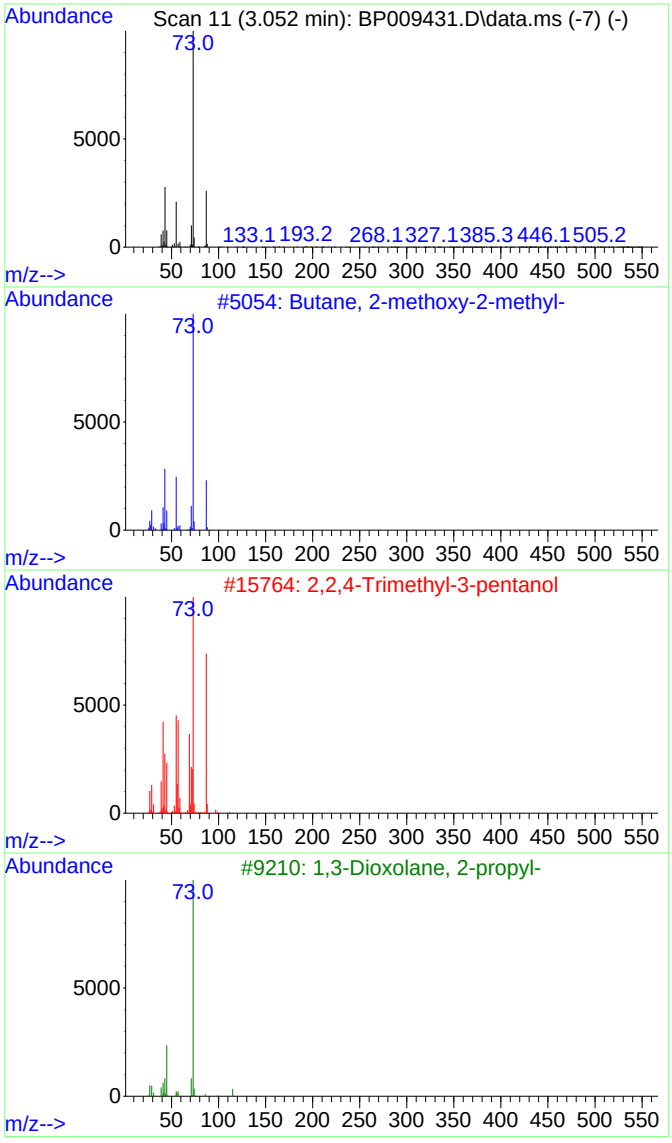
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

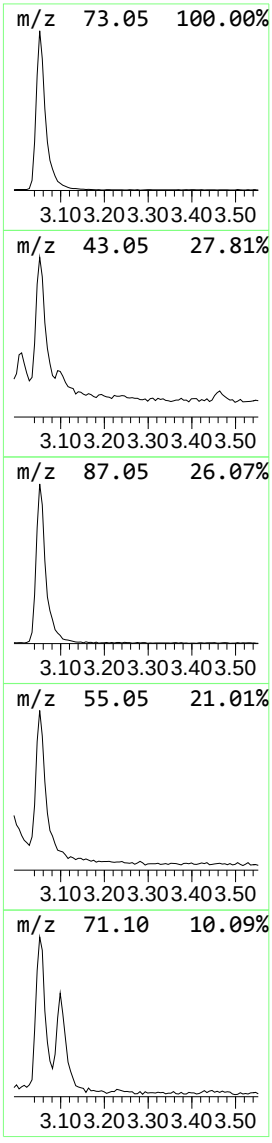
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.052	4.45 ng	528594	1,4-Dichlorobenzene-d4	7.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
Data File : BP009431.D
Acq On : 16 Mar 2022 20:01
Operator : CG/JU
Sample : N1956-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TPK-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

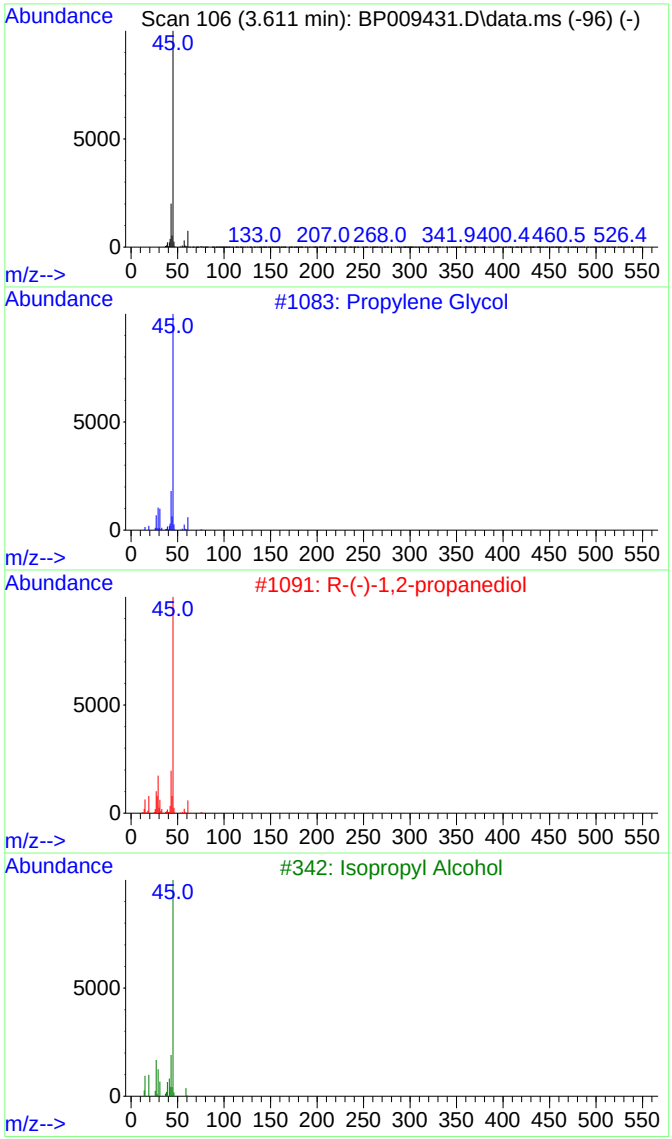
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

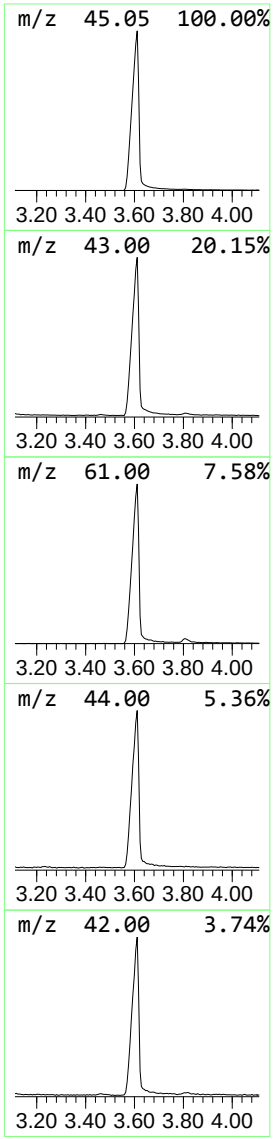
****

Peak Number 2 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.611	73.67 ng	8759390	1,4-Dichlorobenzene-d4	7.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
Data File : BP009431.D
Acq On : 16 Mar 2022 20:01
Operator : CG/JU
Sample : N1956-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TPK-3

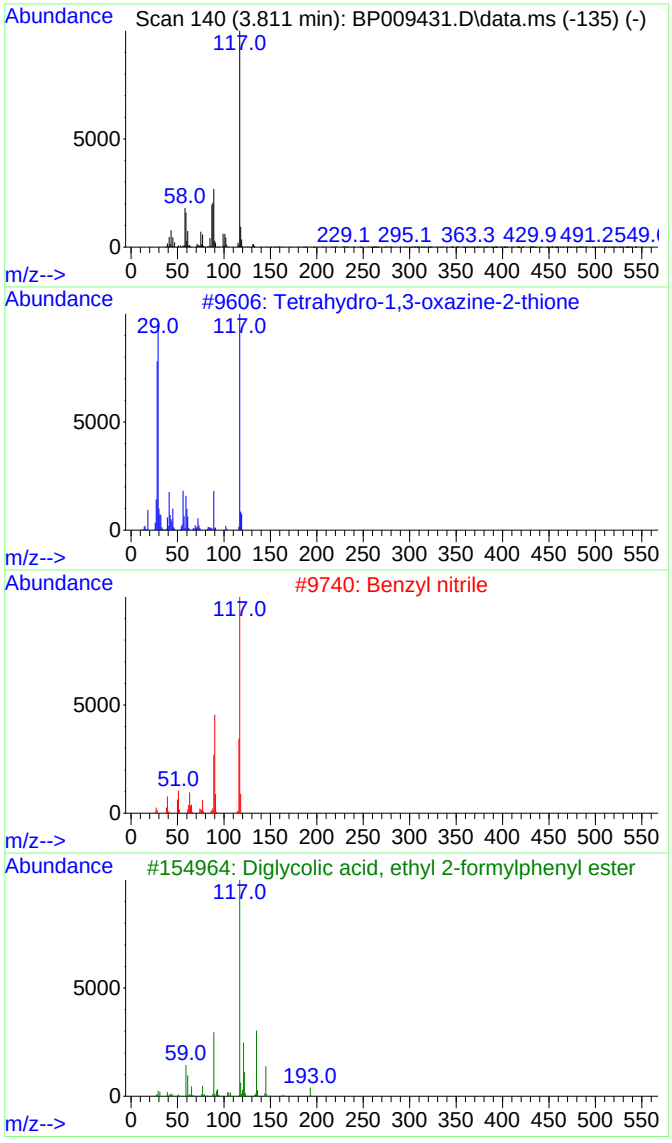
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

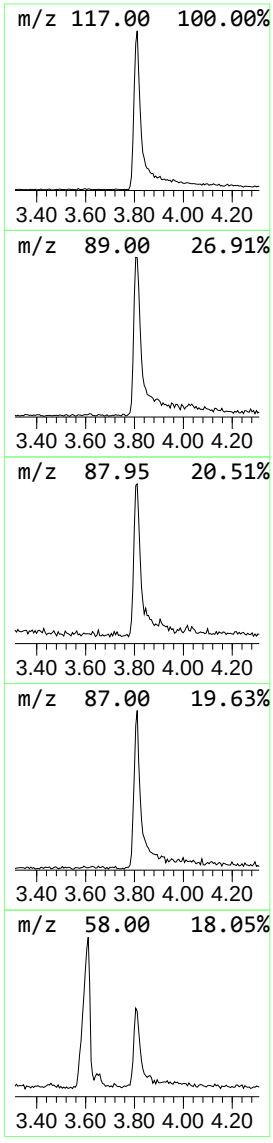
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Tetrahydro-1,3-oxazine-2-th... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.811	3.43 ng	408008	1,4-Dichlorobenzene-d4	7.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrahydro-1,3-oxazine-2-thione	117	C4H7NOS	017374-18-4	50
2	Benzyl nitrile	117	C8H7N	000140-29-4	47
3	Diglycolic acid, ethyl 2-formylp...	266	C13H14O6	1000382-30-6	40
4	Ethyl 3-hydroxyoctanoate	188	C10H20O3	007367-90-0	38
5	2-Thio-2,4-oxazolidinedione	117	C3H3NO2S	002346-24-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP031622\
Data File : BP009431.D
Acq On : 16 Mar 2022 20:01
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Sample : N1956-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TPK-3

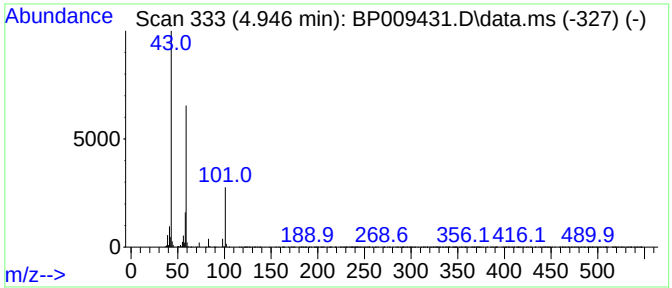
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

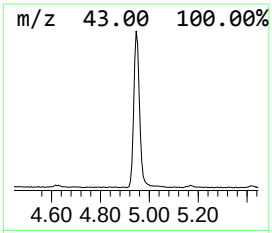
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

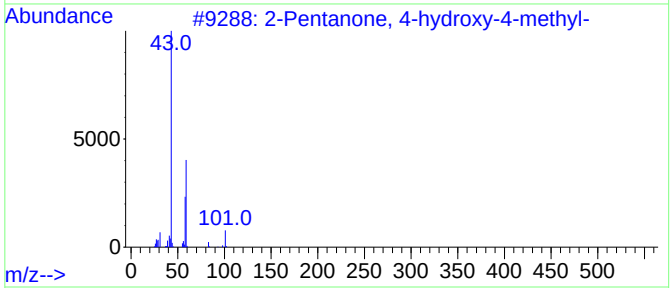
****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

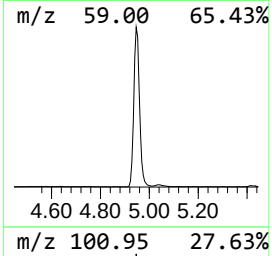
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	7.45 ng	885726	1,4-Dichlorobenzene-d4	7.810

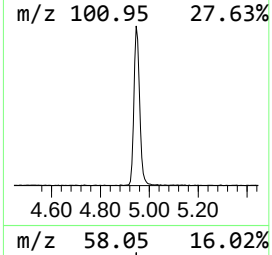
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	28
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17

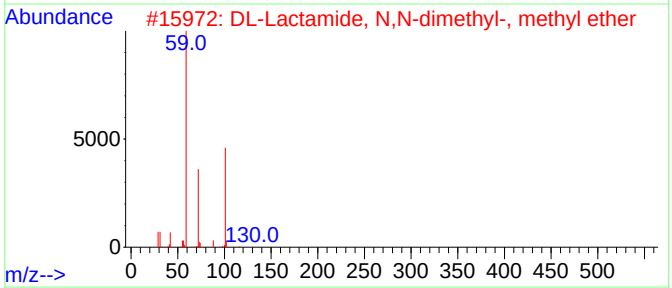


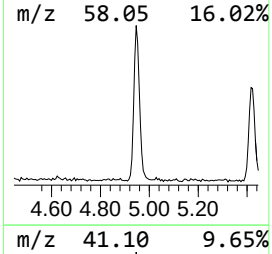


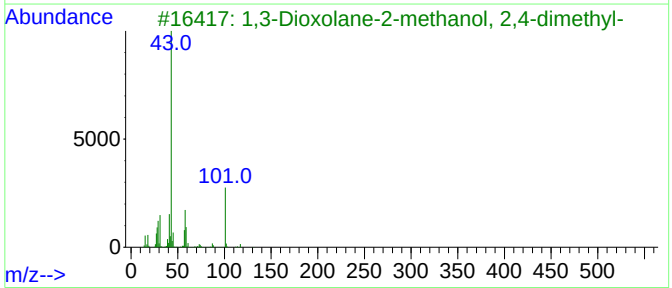


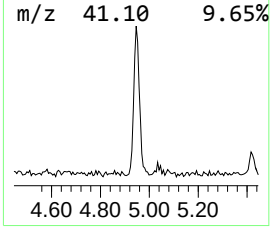












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BNA_P
ClientSampleId :
TPK-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

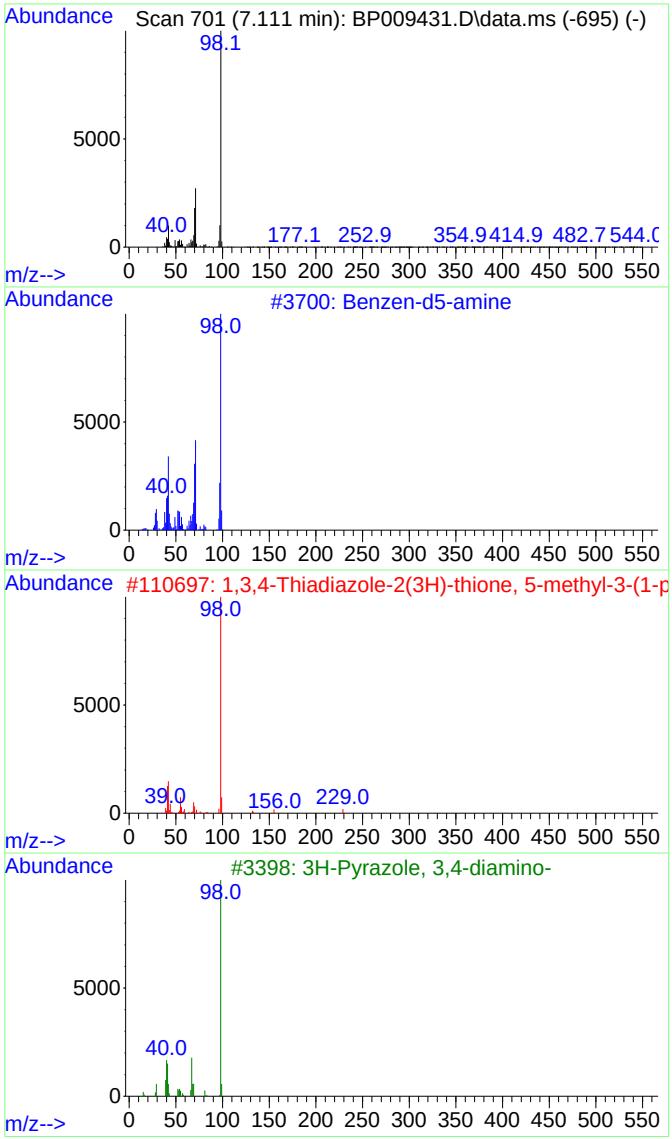
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

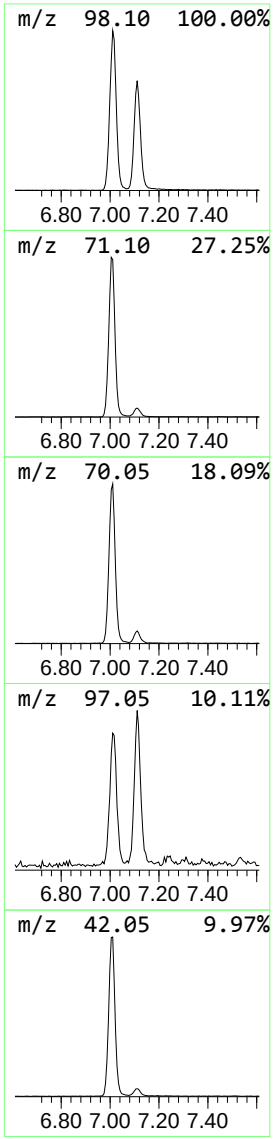
****

Peak Number 5 Benzen-d5-amine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.111	4.20 ng	499434	1,4-Dichlorobenzene-d4	7.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzen-d5-amine	98	C6H2D5N	004165-61-1	56
2	1,3,4-Thiadiazole-2(3H)-thione, ...	229	C9H15N3S2	1000338-18-2	50
3	3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	38
4	1-Methyl-2-piperidinemethanol	129	C7H15NO	020845-34-5	36
5	1H-[1,2,3]Triazole-4-carboxylic ...	307	C12H17N7O3	1000302-67-2	33





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BNA_P
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

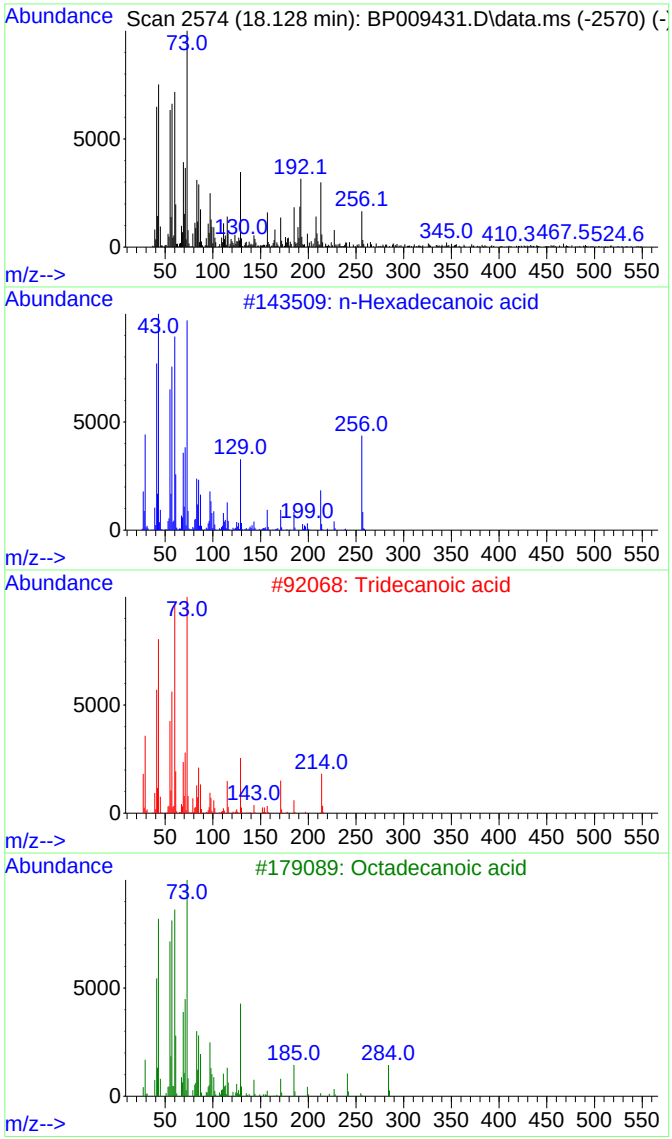
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

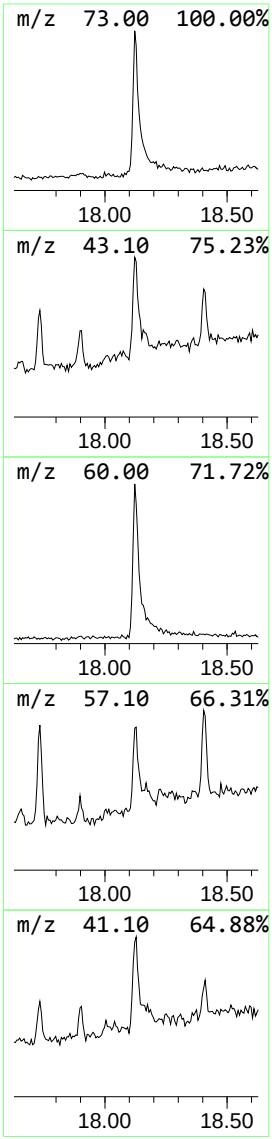
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.128	2.20 ng	618433	Phenanthrene-d10	17.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Octadecanoic acid	284	C18H36O2	000057-11-4	60
4	Docosanoic acid	340	C22H44O2	000112-85-6	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





Tentatively Identified Compound (LSC) summary

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Data File : BP009431.D
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Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.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
Butane, 2-metho...	3.052	4.5	ng	528594	1	7.810	2378110	20.0
Propylene Glycol	3.611	73.7	ng	8759390	1	7.810	2378110	20.0
Tetrahydro-1,3-...	3.811	3.4	ng	408008	1	7.810	2378110	20.0
2-Pentanone, 4-...	4.946	7.5	ng	885726	1	7.810	2378110	20.0
Benzen-d5-amine	7.111	4.2	ng	499434	1	7.810	2378110	20.0
n-Hexadecanoic ...	18.128	2.2	ng	618433	4	17.216	5620930	20.0