LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112221\
Data File : BP008083.D
Acq On : 22 Nov 2021 15:17
Operator : CG/JU
Sample : M4754-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-4-COMP

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-BP111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008083.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	13	rBV	1176019	1469168	22.21%	3.799%
2	3.075	13	15	22	rVB	67222	74456	1.13%	0.193%
3	4.946	327	333	344	rVB	265162	372790	5.63%	0.964%
4	5.410	406	412	427	rBV	2575491	3796978	57.39%	9.819%
5	7.004	672	683	695	rBV	2350878	3895450	58.88%	10.074%
6	7.822	814	822	829	rBV	511179	807355	12.20%	2.088%
7	8.981	1010	1019	1030	rBV	1553809	2546377	38.49%	6.585%
8	10.410	1255	1262	1279	rBV	109374	231764	3.50%	0.599%
9	10.616	1289	1297	1307	rBV	615527	1056152	15.96%	2.731%
10	13.086	1709	1717	1730	rBV	3226998	4921405	74.38%	12.727%
11	14.463	1944	1951	1959	rBV	907936	1328144	20.07%	3.435%
12	15.957	2198	2205	2223	rBV	2590907	3724376	56.29%	9.631%
13	17.222	2412	2420	2425	rBV	1064937	1553527	23.48%	4.017%
14	17.345	2435	2441	2447	rVB4	43173	74062	1.12%	0.192%
15	18.116	2568	2572	2581	rBV	135263	206912	3.13%	0.535%
16	19.239	2759	2763	2768	rVB	56618	74309	1.12%	0.192%
17	19.786	2850	2856	2865	rBV	5292812	6616274	100.00%	17.110%
18	20.468	2968	2972	2977	rBV	86367	106493	1.61%	0.275%
19	21.033	3064	3068	3075	rBV2	419116	599629	9.06%	1.551%
20	21.098	3075	3079	3085	rVB	168721	218231	3.30%	0.564%
21	21.233	3099	3102	3106	rVB	99567	107085	1.62%	0.277%
22	21.315	3110	3116	3120	rBV	1532731	2066600	31.24%	5.344%
23	21.351	3120	3122	3128	rVB	141683	181316	2.74%	0.469%
24	21.474	3140	3143	3147	rVB	105465	123661	1.87%	0.320%
25	22.427	3301	3305	3314	rVB2	327889	484804	7.33%	1.254%
26	23.715	3518	3524	3532	rVB2	1002695	2032181	30.71%	5.255%

Sum of corrected areas: 38669499

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Misc :
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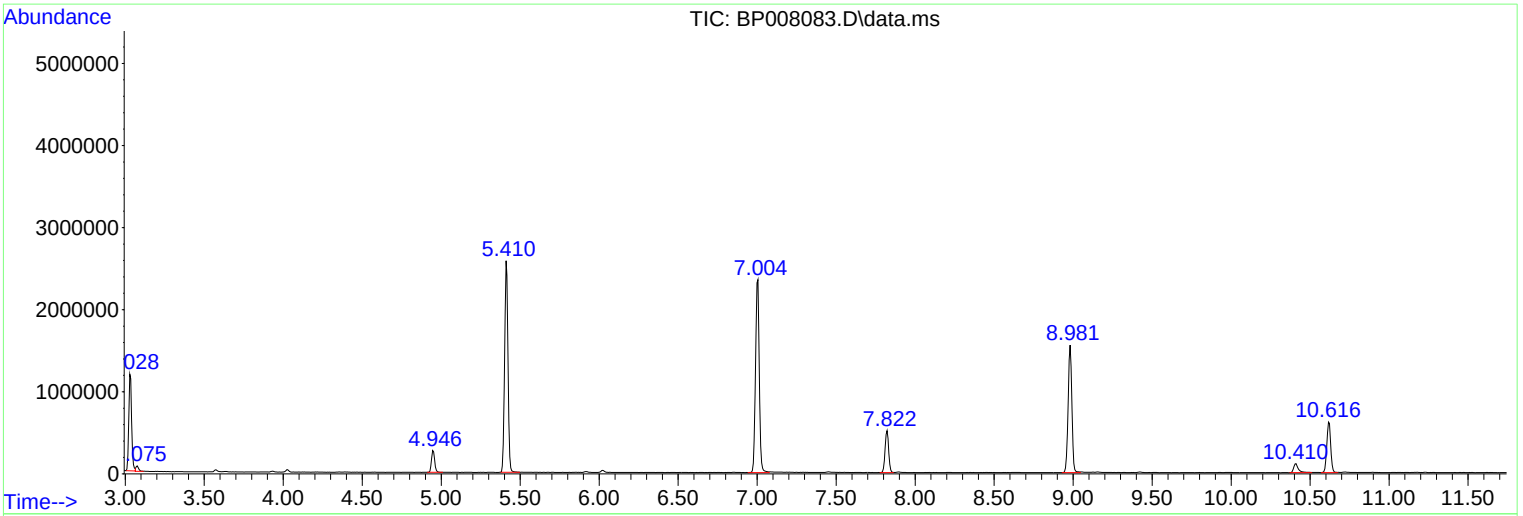
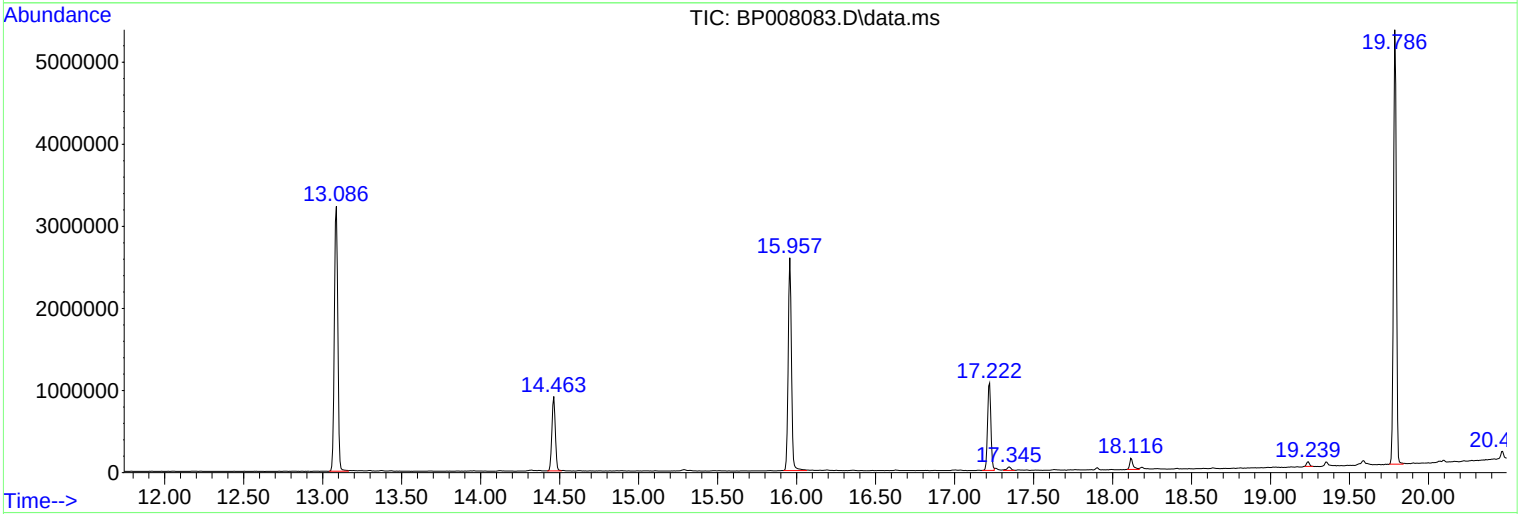
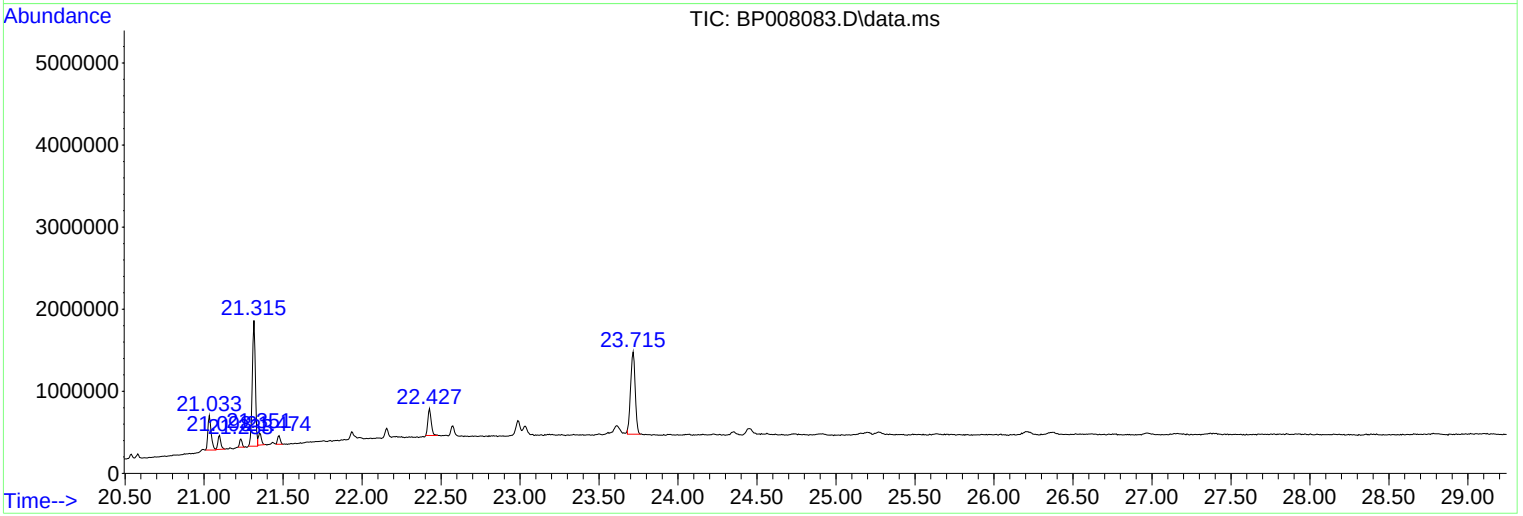
Instrument :
BNA_P
ClientSampleId :
TP-4-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

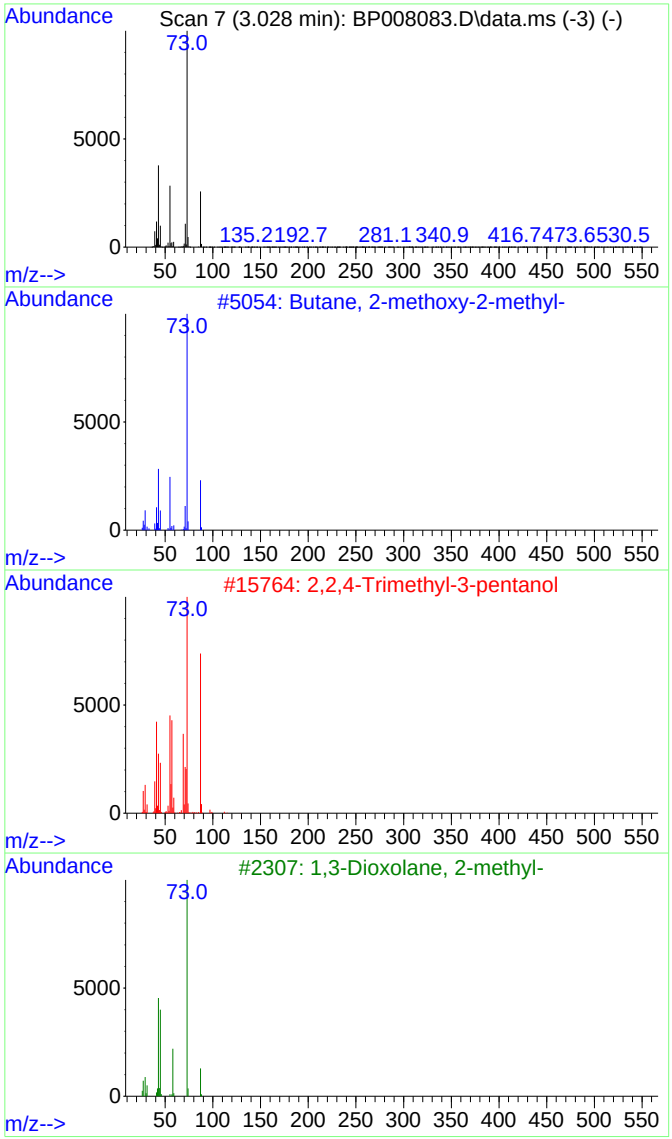
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

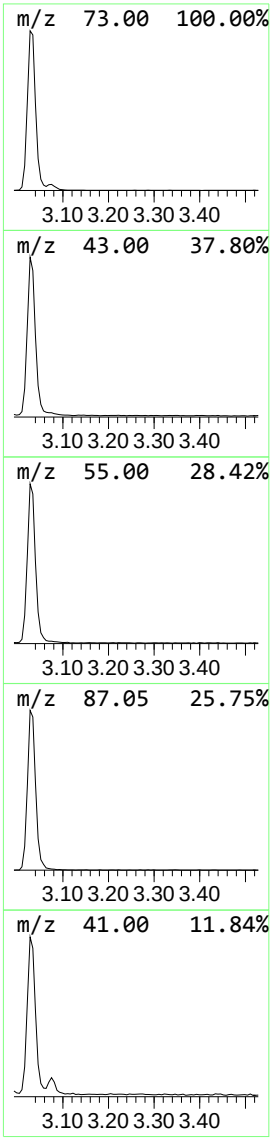
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	36.39 ng	1469170	1,4-Dichlorobenzene-d4	7.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Acq On : 22 Nov 2021 15:17
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Misc :
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Instrument :
BNA_P
ClientSampleId :
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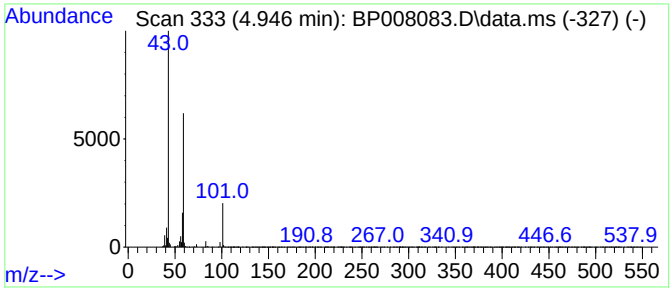
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

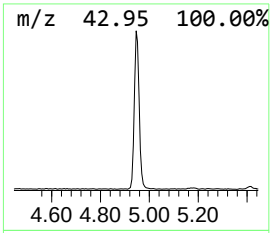
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

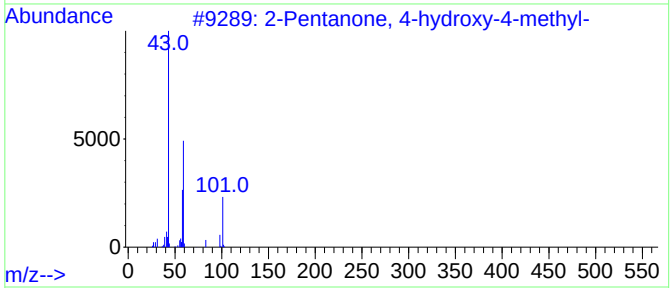
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

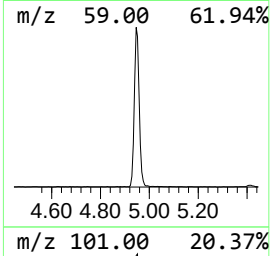
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	9.23 ng	372790	1,4-Dichlorobenzene-d4	7.822

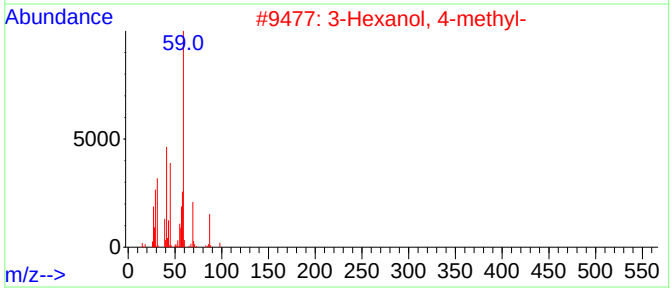
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10

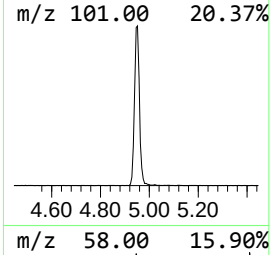


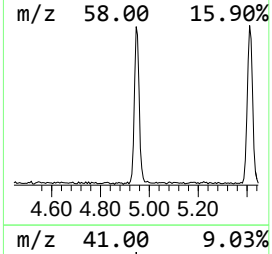


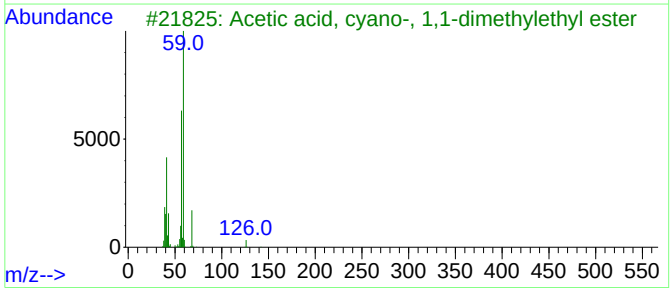


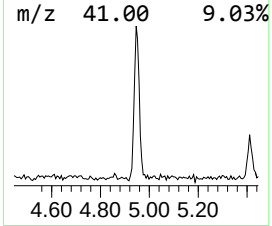












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Data File : BP008083.D
Acq On : 22 Nov 2021 15:17
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Sample : M4754-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-4-COMP

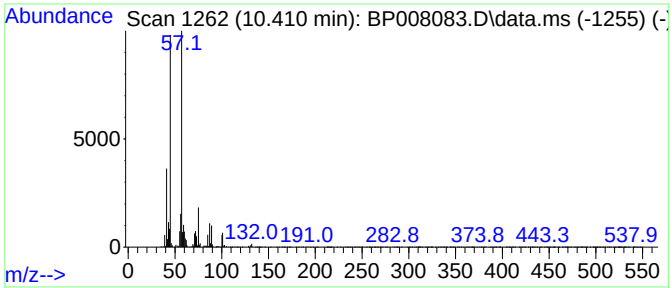
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

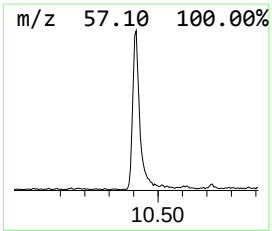
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

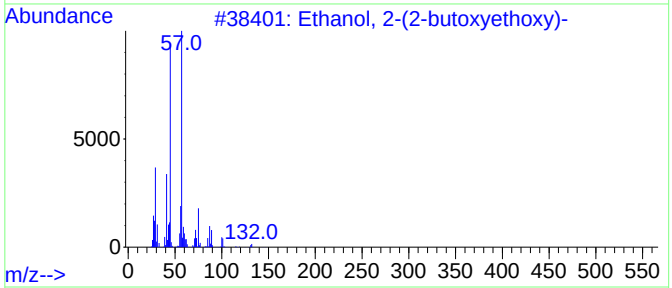
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

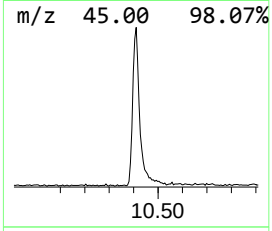
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.410	4.39 ng	231764	Naphthalene-d8	10.616

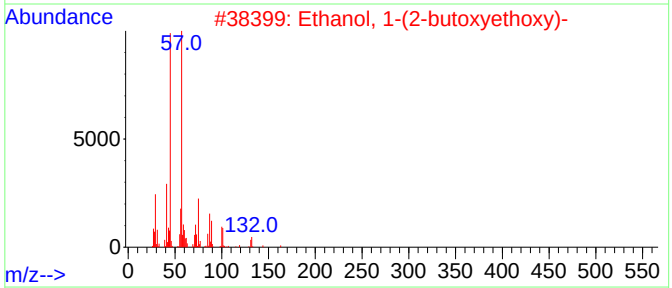
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4	Pentaethylene glycol	238	C10H22O6	004792-15-8	50
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50

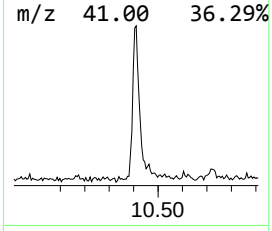


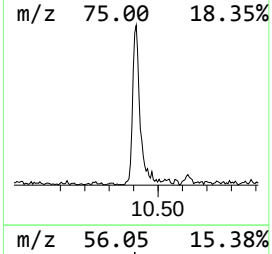


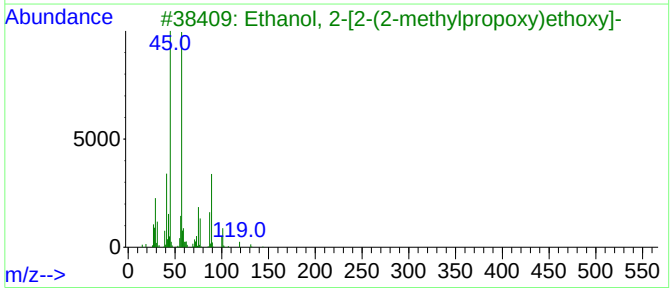


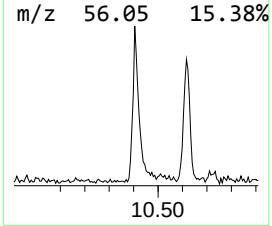












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

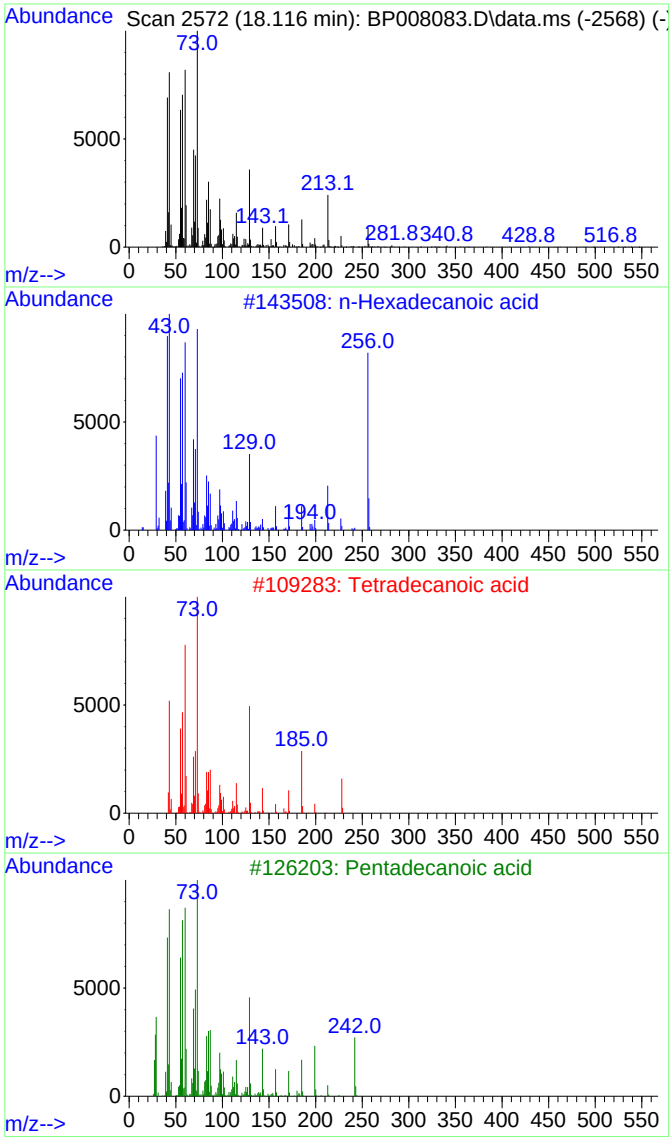
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

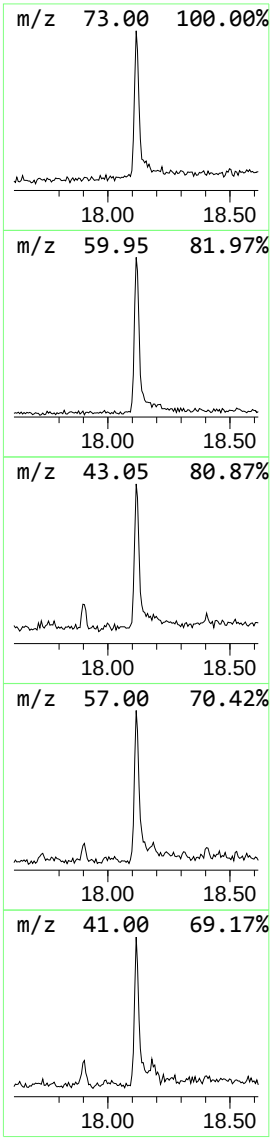
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.116	2.66 ng	206912	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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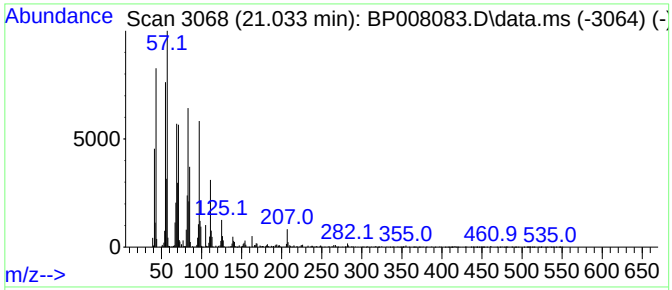
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

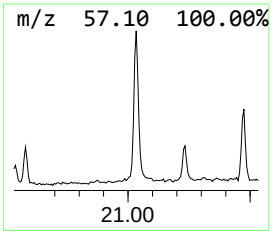
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

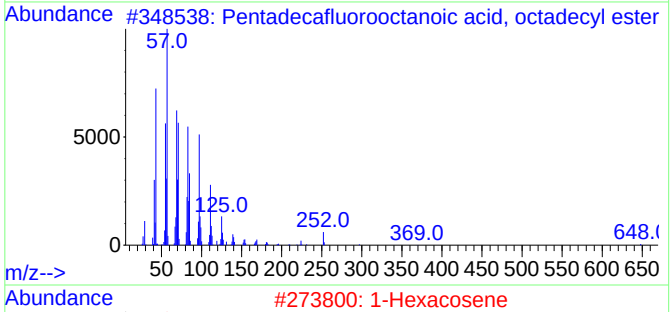
****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 3

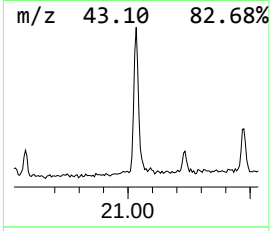
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	5.80 ng	599629	Chrysene-d12	21.316

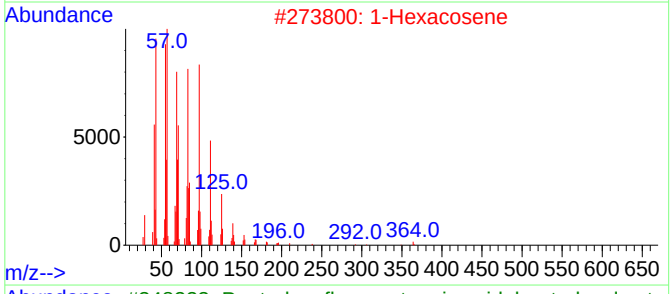
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	Pentadecafluorooctanoic acid, he...	652	C25H35F15O2	1000406-04-7	91
4	Heneicosyl pentafluoropropionate	458	C24H43F5O2	1000351-81-1	91
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91

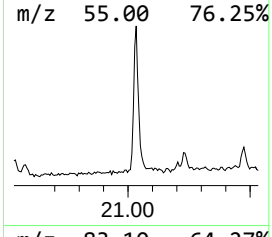


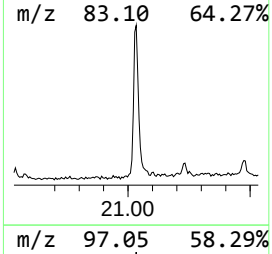


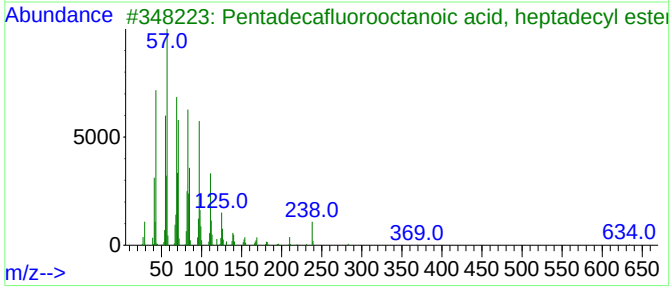


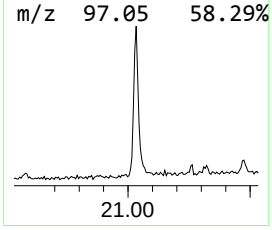












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Data File : BP008083.D
Acq On : 22 Nov 2021 15:17
Operator : CG/JU
Sample : M4754-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-4-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

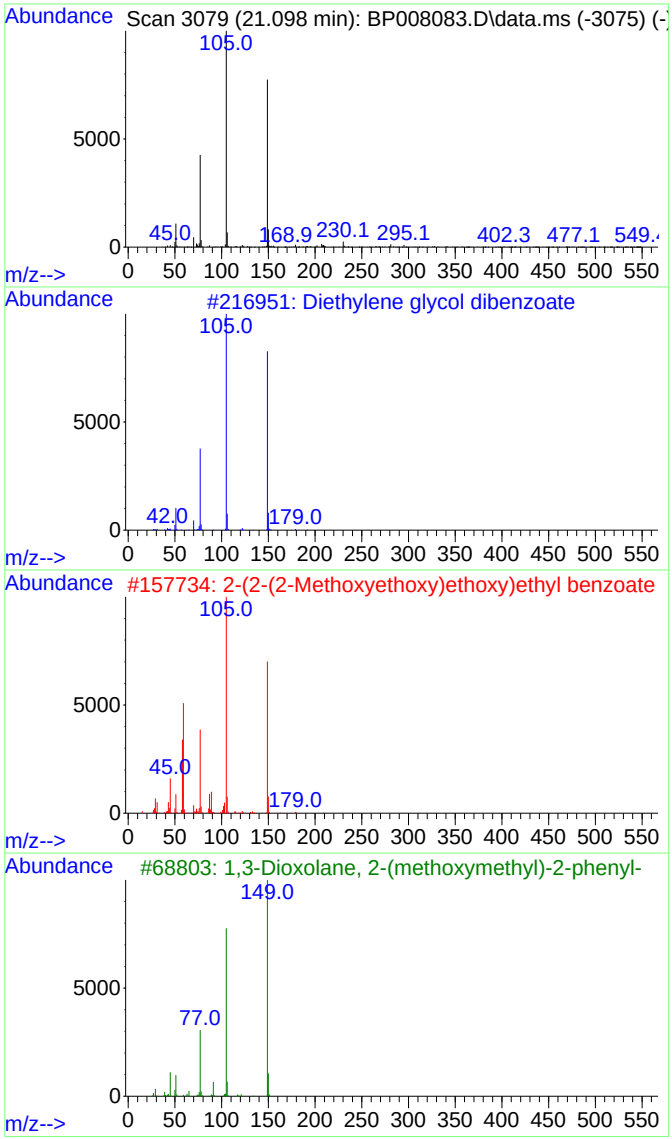
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

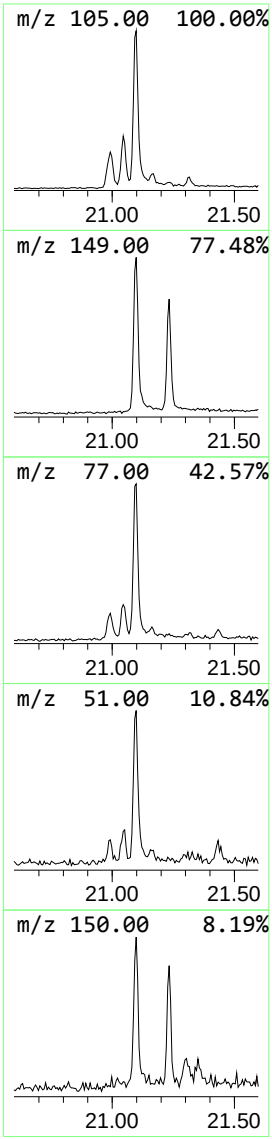
****

Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.098	2.11 ng	218231	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	78
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
4	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	56
5	2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112221\
Data File : BP008083.D
Acq On : 22 Nov 2021 15:17
Operator : CG/JU
Sample : M4754-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-4-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

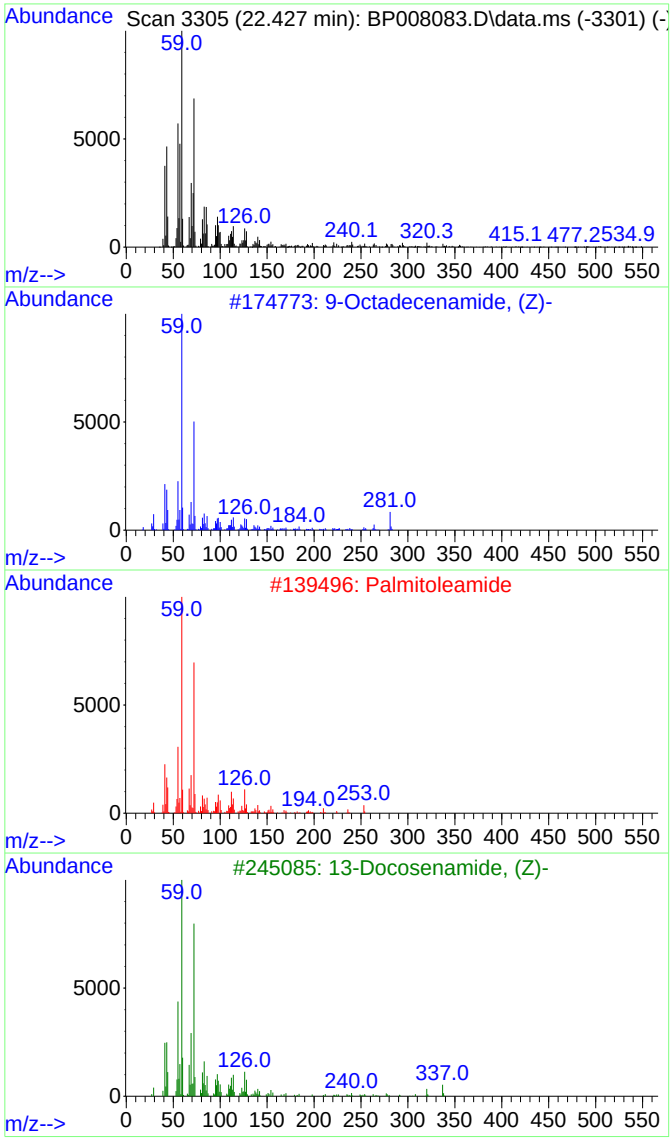
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

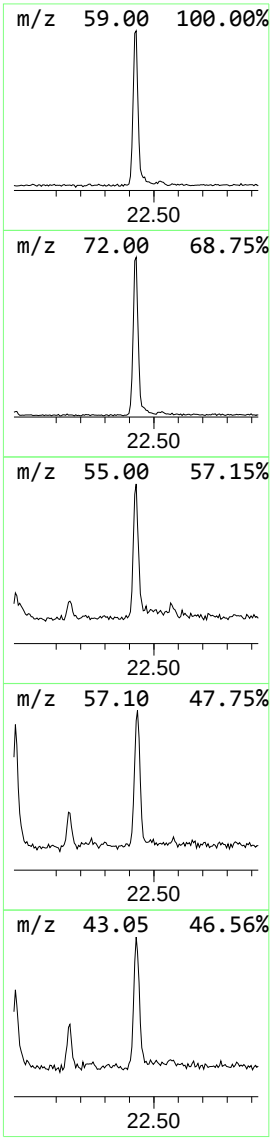
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.427	4.69 ng	484804	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	Palmitoleamide	253	C16H31NO	106010-22-4	80
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	78
4	Tetradecanamide	227	C14H29NO	000638-58-4	59
5	3-Tetradecanone	212	C14H28O	000629-23-2	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112221\
Data File : BP008083.D
Acq On : 22 Nov 2021 15:17
Operator : CG/JU
Sample : M4754-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-4-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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...	3.028	36.4	ng	1469170	1	7.822	807355	20.0
2-Pentanone, 4-...	4.946	9.2	ng	372790	1	7.822	807355	20.0
Ethanol, 2-(2-b...	10.410	4.4	ng	231764	2	10.616	1056150	20.0
n-Hexadecanoic ...	18.116	2.7	ng	206912	4	17.222	1553530	20.0
Pentadecafluoro...	21.033	5.8	ng	599629	5	21.316	2066600	20.0
Diethylene glyc...	21.098	2.1	ng	218231	5	21.316	2066600	20.0
9-Octadecenamid...	22.427	4.7	ng	484804	5	21.316	2066600	20.0