Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021579.D
Acq On : 20 Aug 2024 19:34
Operator : RC/JU
Sample : P3643-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524-FD

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-BP081324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP021579.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	23	rVB	2905573	3484073	30.73%	4.913%
2	3.546	91	95	105	rVB	155698	204846	1.81%	0.289%
3	4.940	327	332	343	rVB	205086	289792	2.56%	0.409%
4	5.399	403	410	420	rBV	3561059	5254734	46.35%	7.409%
5	6.969	669	677	687	rBV	3545792	5641352	49.76%	7.954%
6	7.805	810	819	826	rBV	1209312	1894196	16.71%	2.671%
7	8.946	1006	1013	1023	rBV	1986186	3365087	29.68%	4.745%
8	9.510	1102	1109	1116	rBV	77650	132771	1.17%	0.187%
9	10.593	1284	1293	1302	rBV	1490216	2664865	23.50%	3.757%
10	11.328	1411	1418	1429	rBV	186011	356022	3.14%	0.502%
11	13.063	1705	1713	1728	rBV	3964986	6524921	57.55%	9.200%
12	14.457	1940	1950	1958	rBV	2522655	3788463	33.42%	5.342%
13	14.687	1980	1989	2000	rVB5	89690	243225	2.15%	0.343%
14	15.975	2201	2208	2228	rBV	4153264	6551808	57.79%	9.238%
15	17.269	2421	2428	2435	rBV	2804822	4883781	43.08%	6.886%
16	18.210	2582	2588	2599	rBV	463793	758841	6.69%	1.070%
17	19.398	2786	2790	2797	rBV	218538	327092	2.89%	0.461%
18	19.545	2811	2815	2823	rBV2	188956	299490	2.64%	0.422%
19	19.775	2850	2854	2860	rVB2	126558	209047	1.84%	0.295%
20	19.992	2884	2891	2900	rBV	7394076	11337583	100.00%	15.986%
21	21.410	3127	3132	3142	rBV	655829	959030	8.46%	1.352%
22	21.733	3180	3187	3193	rBV	3653296	5904893	52.08%	8.326%
23	25.186	3764	3774	3786	rVB2	2020680	5846678	51.57%	8.244%

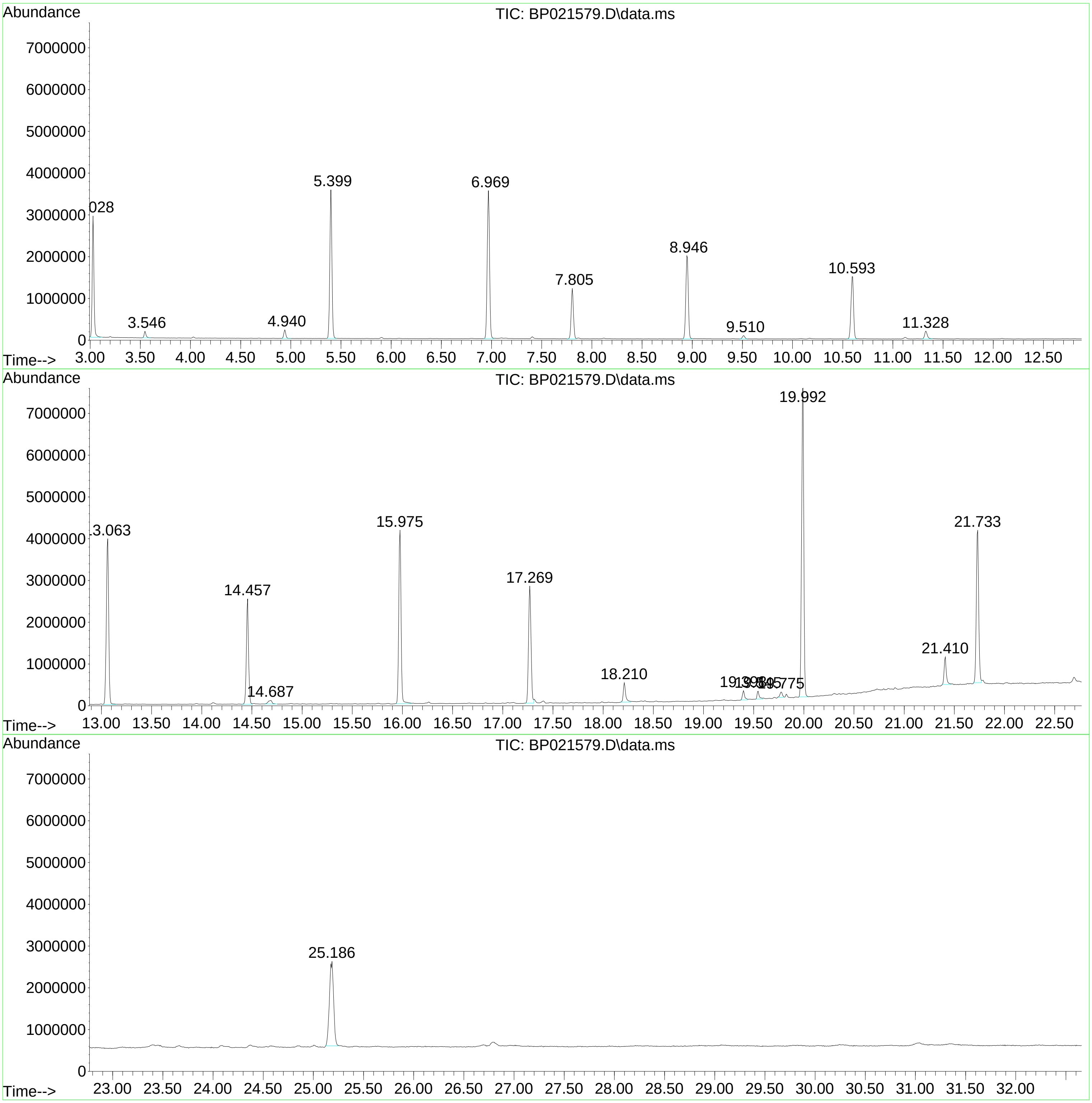
Sum of corrected areas: 70922590

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021579.D
Acq On : 20 Aug 2024 19:34
Operator : RC/JU
Sample : P3643-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524-FD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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\BP082024\
Data File : BP021579.D
Acq On : 20 Aug 2024 19:34
Operator : RC/JU
Sample : P3643-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524-FD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

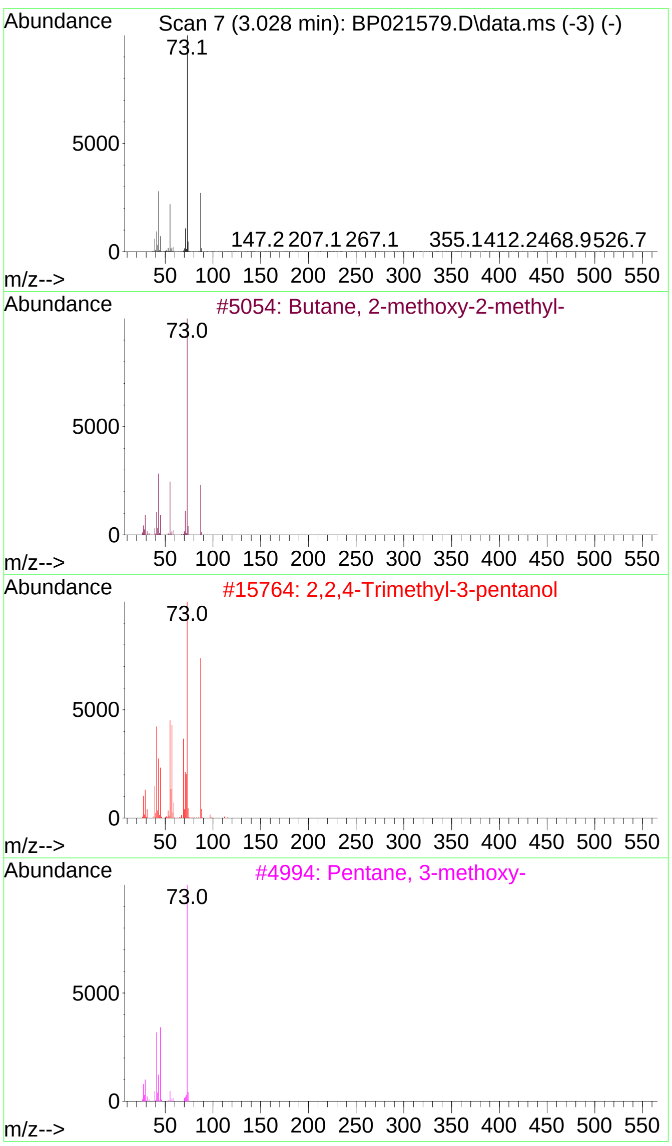
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

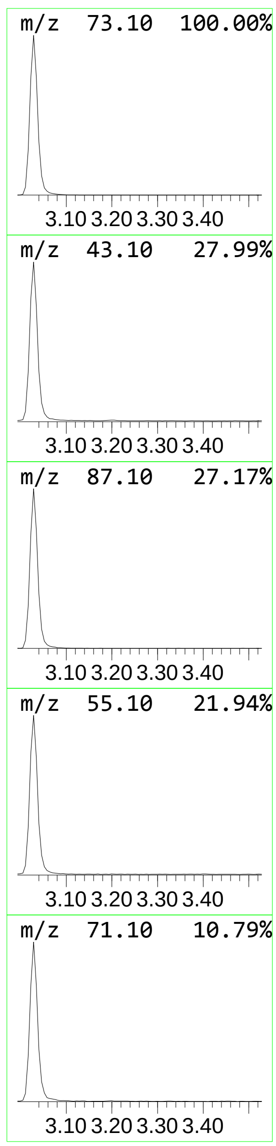
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	36.79 ng	3484070	1,4-Dichlorobenzene-d4	7.805

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	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021579.D
Acq On : 20 Aug 2024 19:34
Operator : RC/JU
Sample : P3643-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524-FD

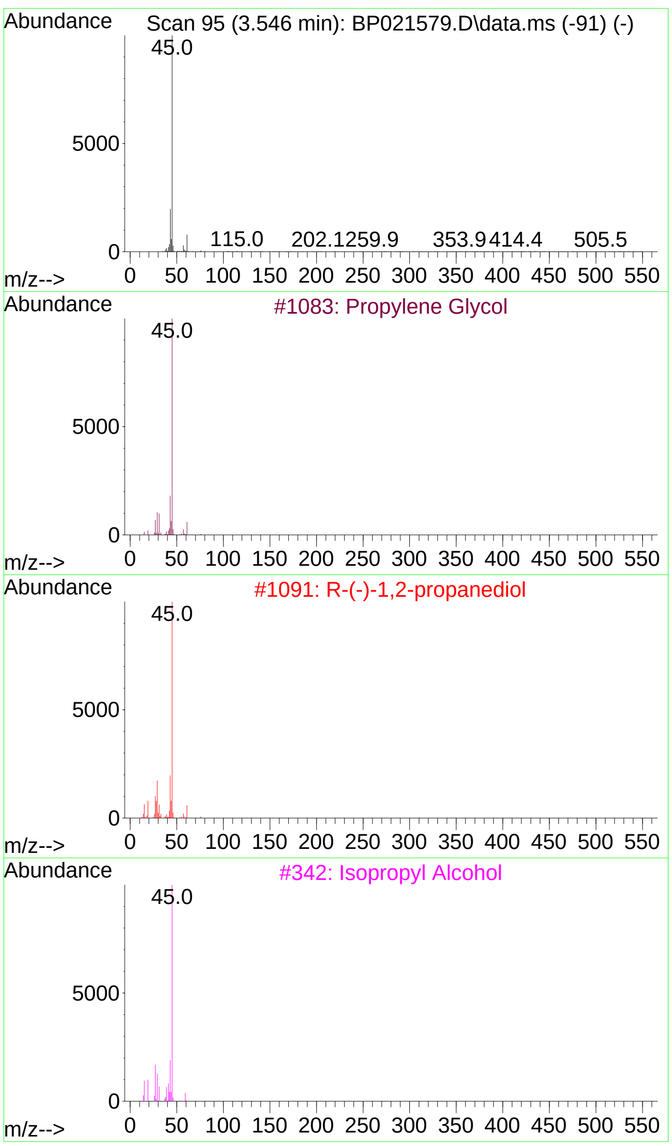
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

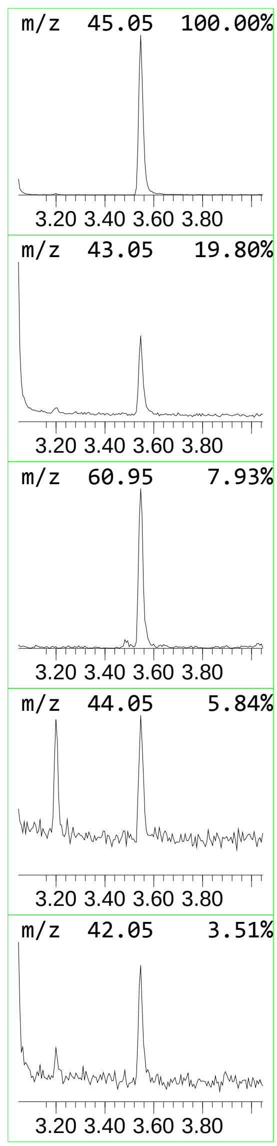
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.546	2.16 ng	204846	1,4-Dichlorobenzene-d4	7.805

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021579.D
Acq On : 20 Aug 2024 19:34
Operator : RC/JU
Sample : P3643-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524-FD

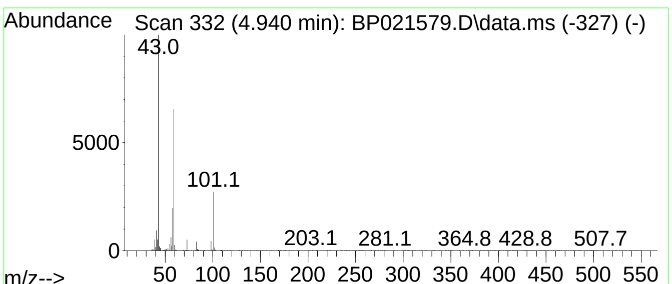
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

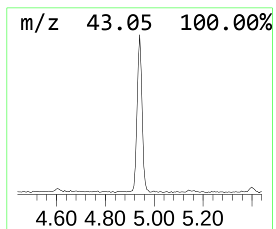
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

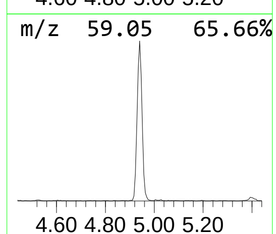
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

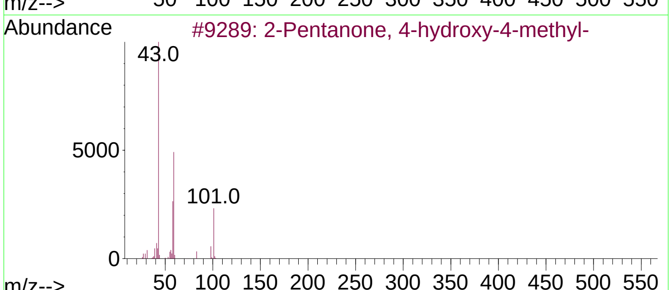
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	3.06 ng	289792	1,4-Dichlorobenzene-d4	7.805

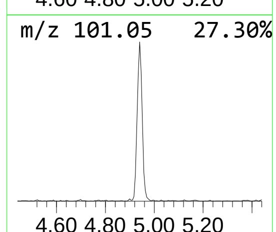
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	37
3	(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	33
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	32
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	27

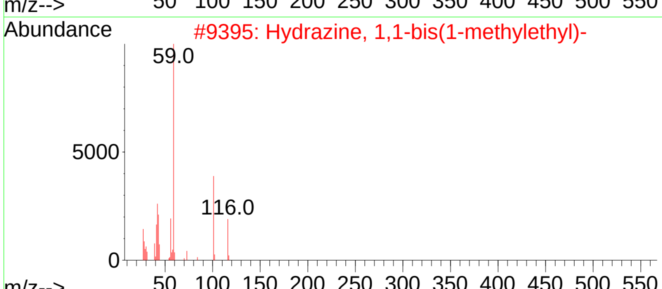


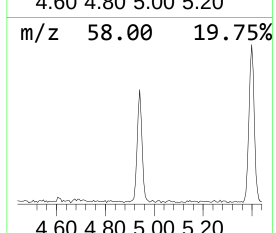


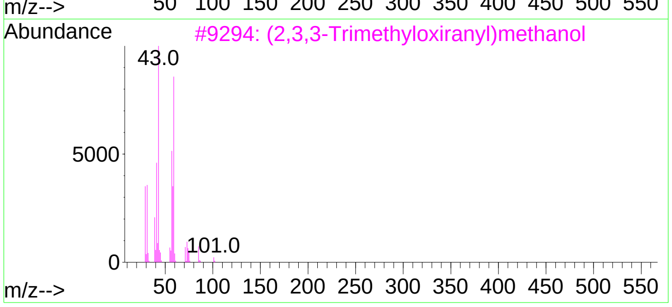


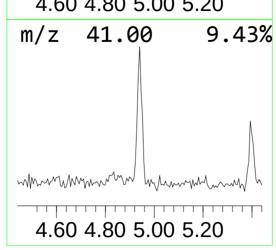












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021579.D
Acq On : 20 Aug 2024 19:34
Operator : RC/JU
Sample : P3643-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524-FD

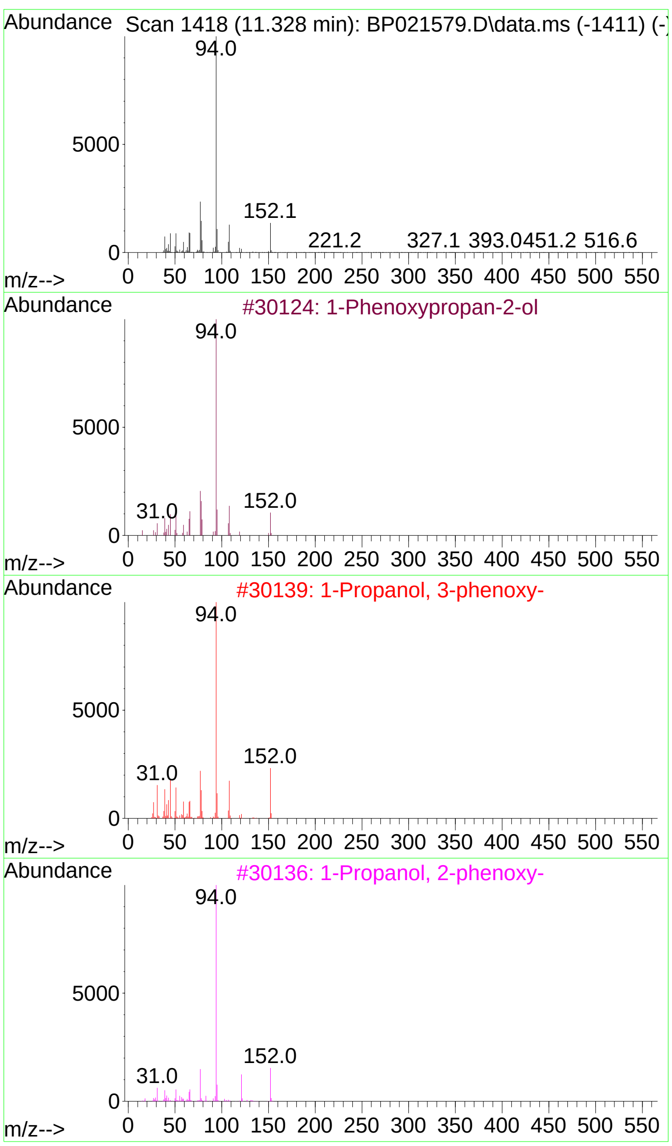
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

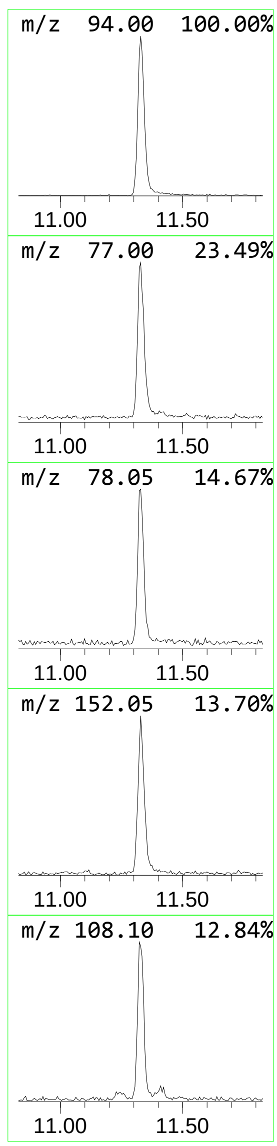
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.328	2.67 ng	356022	Naphthalene-d8	10.599

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	DL-Gabaculine	139	C7H9NO2	059556-18-2	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





Library Search Compound Report

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Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021579.D
Acq On    : 20 Aug 2024  19:34
Operator  : RC/JU
Sample    : P3643-14
Misc      :
ALS Vial  : 6   Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title  : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

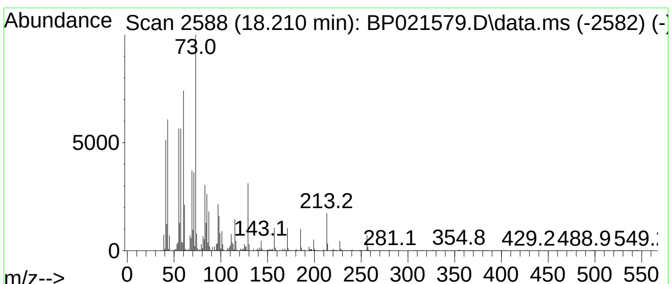
Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524-FD

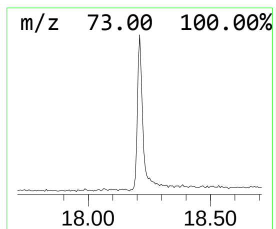
****

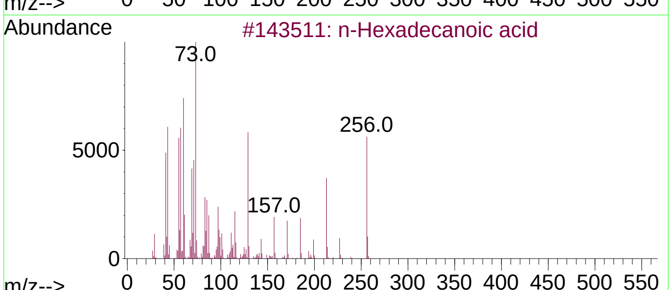
Peak Number 5 n-Hexadecanoic acid   Concentration Rank 3

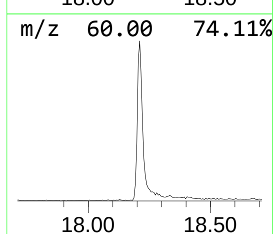
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.210	3.11 ng	758841	Phenanthrene-d10	17.269

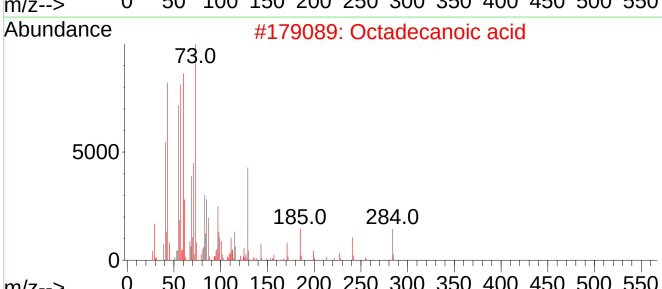
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59

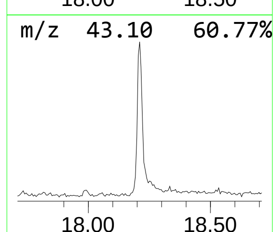


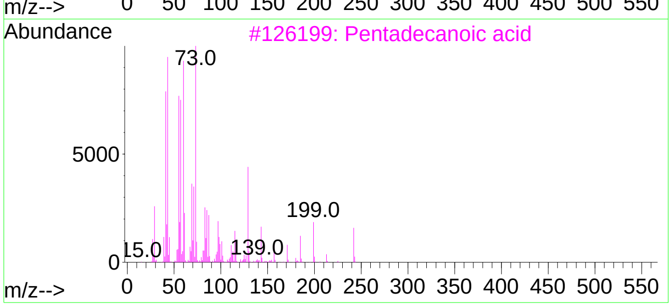


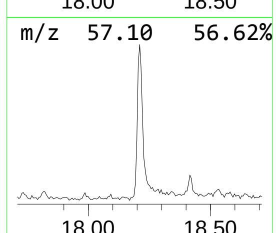


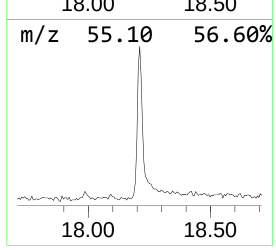












Library Search Compound Report

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Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021579.D
Acq On    : 20 Aug 2024  19:34
Operator  : RC/JU
Sample    : P3643-14
Misc      :
ALS Vial  : 6   Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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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Instrument :
BNA_P
ClientSampleId :
921-J-SD-0.5-1.0-081524-FD

```
*********************************************************************
Peak Number  6  Dichloroacetic acid, heptad...  Concentration Rank  2

  R.T.     EstConc          Area       Relative to ISTD         R.T.
---------------------------------------------------------------------
 21.410    3.25 ng         959030   Chrysene-d12               21.733

 Hit# of  5    Tentative ID               MW  MolForm       CAS#       Qual
---------------------------------------------------------------------
 1 Dichloroacetic acid, heptadecyl ... 366 C19H36Cl2O2    1000282-98-2 91
 2 n-Nonadecanol-1                     284 C19H40O        001454-84-8 90
 3 Trichloroacetic acid, hexadecyl ... 386 C18H33Cl3O2    074339-54-1 90
 4 3-Eicosene, (E)-                    280 C20H40         074685-33-9 90
 5 1-Heneicosanol                      312 C21H44O        015594-90-8 90
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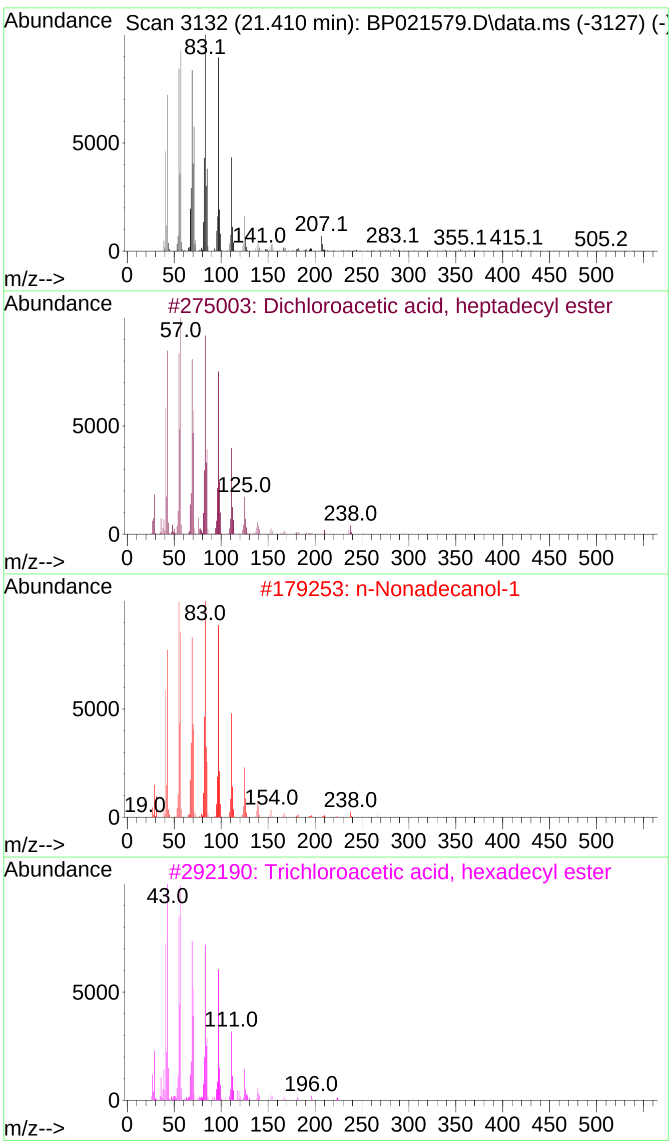

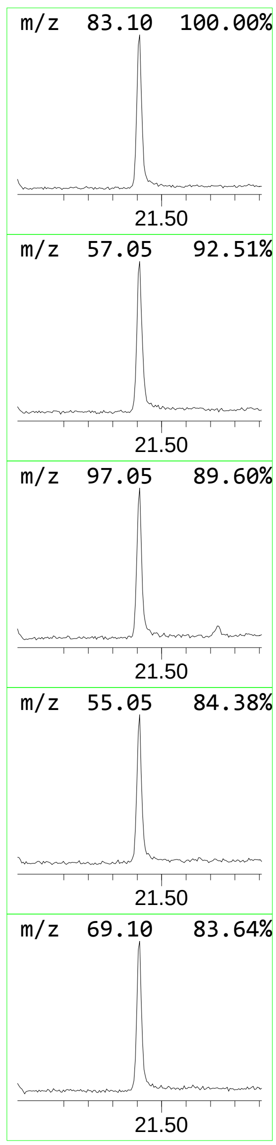

Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082024\
Data File : BP021579.D
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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	36.8	ng	3484070	1	7.805	1894200	20.0
Propylene Glycol	3.546	2.2	ng	204846	1	7.805	1894200	20.0
2-Pentanone, 4-...	4.940	3.1	ng	289792	1	7.805	1894200	20.0
1-Phenoxypropan...	11.328	2.7	ng	356022	2	10.599	2664870	20.0
n-Hexadecanoic ...	18.210	3.1	ng	758841	4	17.269	4883780	20.0
Dichloroacetic ...	21.410	3.3	ng	959030	5	21.733	5904890	20.0