LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
Data File : BP019701.D
Acq On : 14 Feb 2024 14:57
Operator : MA/JU
Sample : P1453-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

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-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019701.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.628	88	92	98	rBV	38008	55110	1.07%	0.240%
2	5.022	319	329	337	rBV	71614	108746	2.11%	0.473%
3	5.475	400	406	420	rBV	1277016	1968978	38.20%	8.572%
4	6.899	640	648	666	rBV3	32870	160376	3.11%	0.698%
5	7.075	670	678	696	rVV	1211192	1990648	38.62%	8.667%
6	7.905	809	819	827	rVB	262897	428234	8.31%	1.864%
7	9.075	1009	1018	1030	rBV	768410	1342946	26.05%	5.847%
8	10.705	1286	1295	1306	rBV	310393	552015	10.71%	2.403%
9	12.863	1655	1662	1668	rBV2	32807	65557	1.27%	0.285%
10	12.934	1668	1674	1687	rVB	93236	193754	3.76%	0.844%
11	13.163	1703	1713	1729	rBV	1957629	3043672	59.05%	13.251%
12	14.540	1938	1947	1962	rBV	442683	728772	14.14%	3.173%
13	16.034	2193	2201	2223	rBV	1671379	2750499	53.36%	11.975%
14	17.292	2407	2415	2427	rBV	621910	947853	18.39%	4.127%
15	18.192	2562	2568	2579	rBV	409272	586976	11.39%	2.556%
16	19.428	2774	2778	2789	rBV	175015	237005	4.60%	1.032%
17	19.863	2846	2852	2859	rBV	4149931	5154800	100.00%	22.443%
18	20.545	2965	2968	2974	rVB	48104	58544	1.14%	0.255%
19	21.110	3060	3064	3069	rBV2	211390	259721	5.04%	1.131%
20	21.386	3106	3111	3118	rBV	900043	1146772	22.25%	4.993%
21	23.804	3516	3522	3530	rVB	565553	1187583	23.04%	5.170%

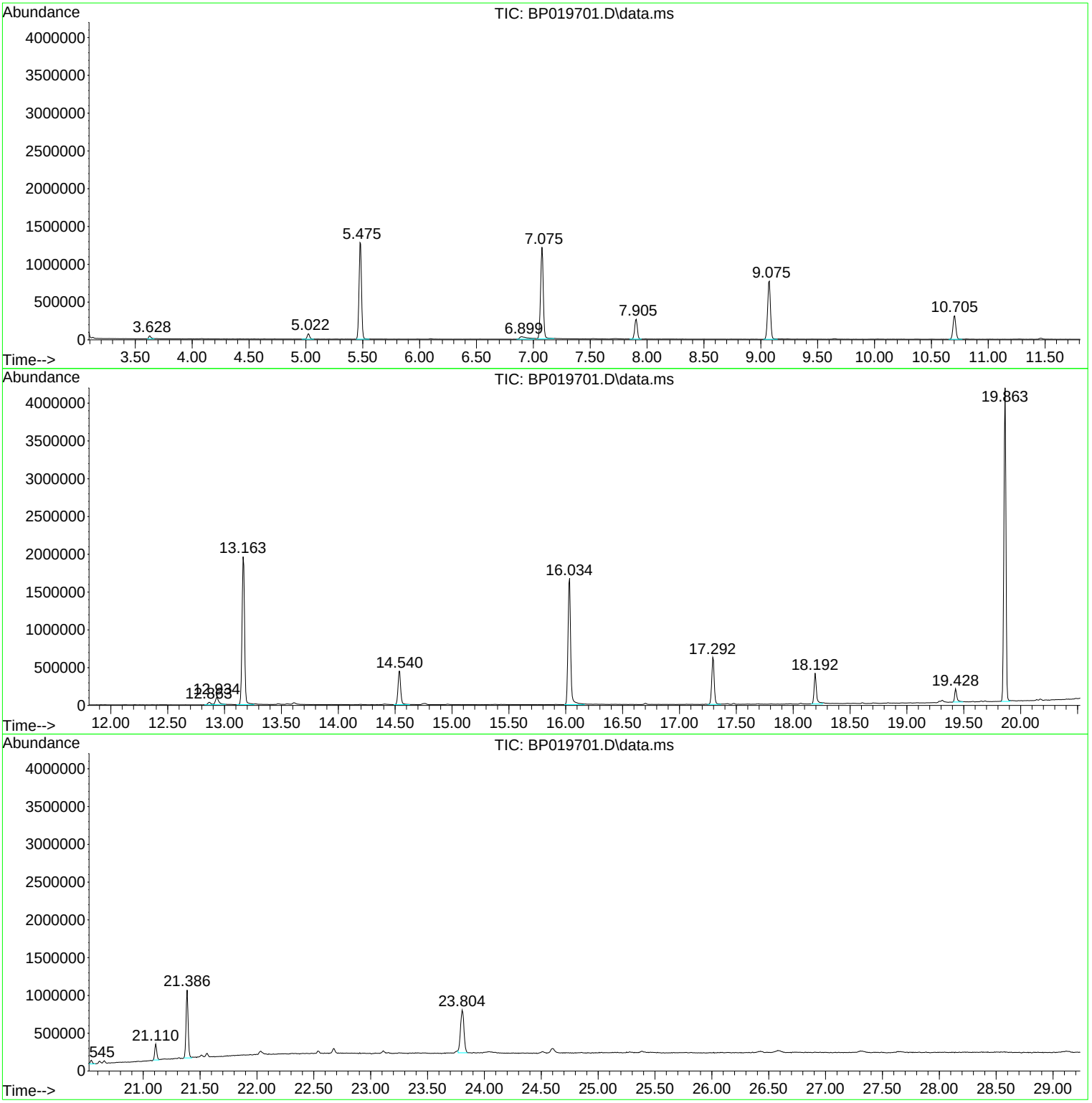
Sum of corrected areas: 22968561

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
Data File : BP019701.D
Acq On : 14 Feb 2024 14:57
Operator : MA/JU
Sample : P1453-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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\BP021424\
Data File : BP019701.D
Acq On : 14 Feb 2024 14:57
Operator : MA/JU
Sample : P1453-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

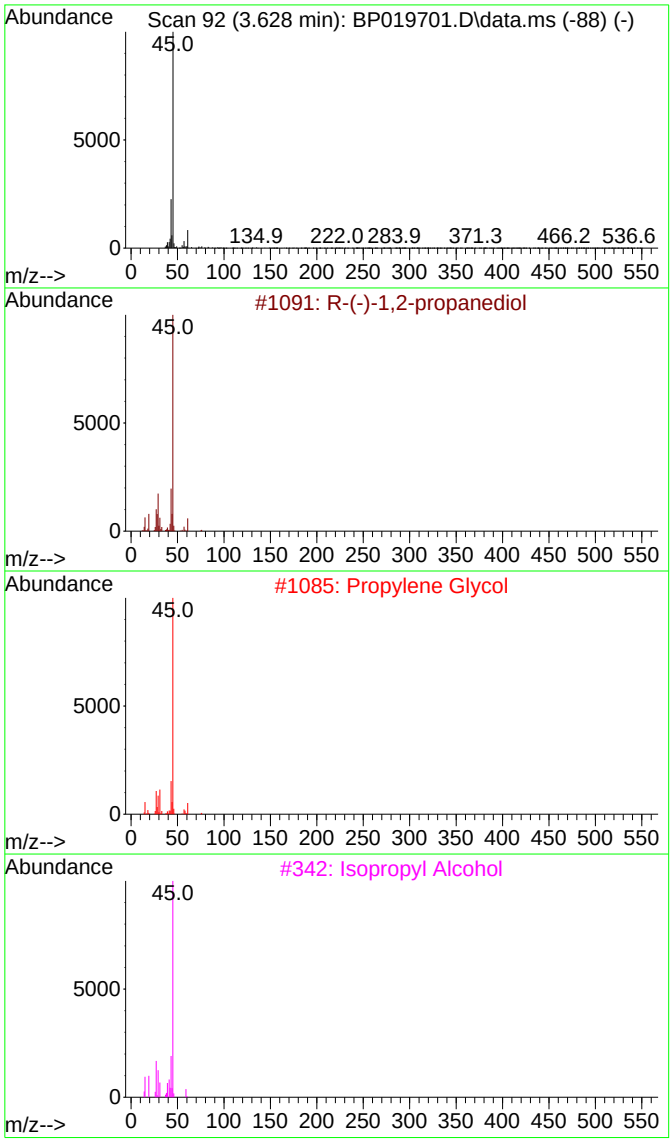
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

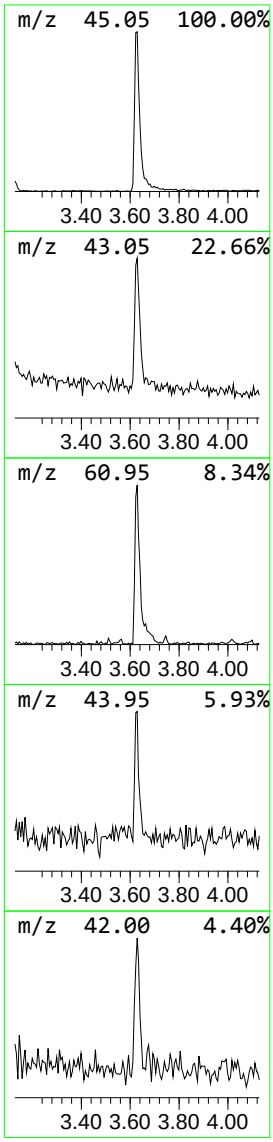
****

Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.628	2.57 ng	55110	1,4-Dichlorobenzene-d4	7.905

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
2	Propylene Glycol	76	C3H8O2	000057-55-6	56
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
5	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	39





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Data File : BP019701.D
Acq On : 14 Feb 2024 14:57
Operator : MA/JU
Sample : P1453-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

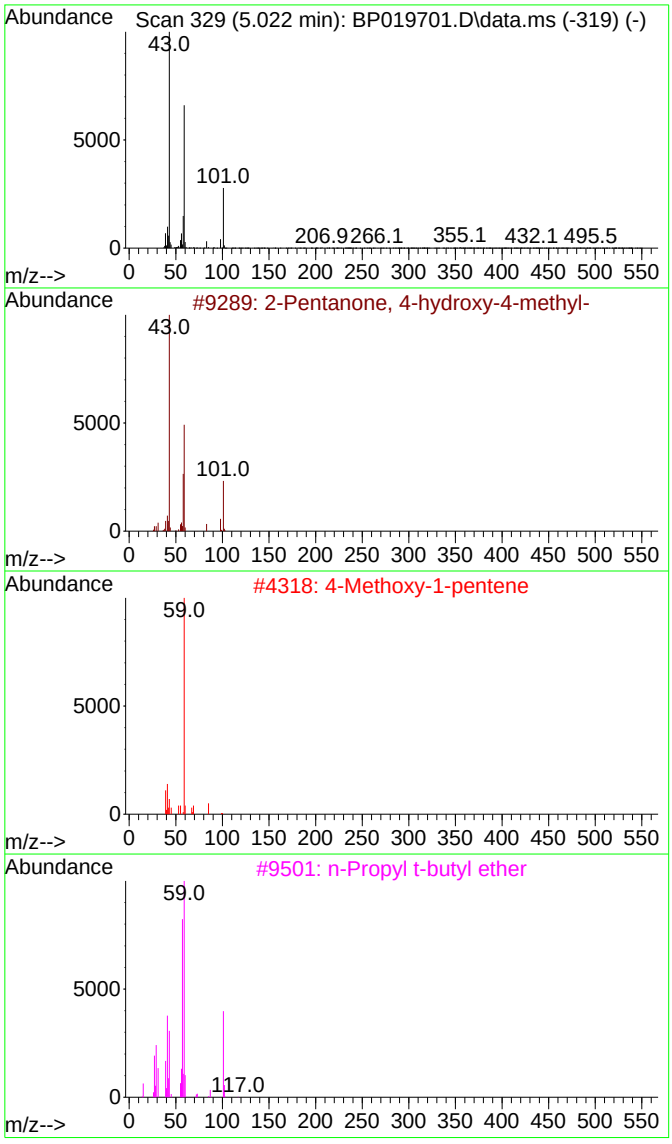
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

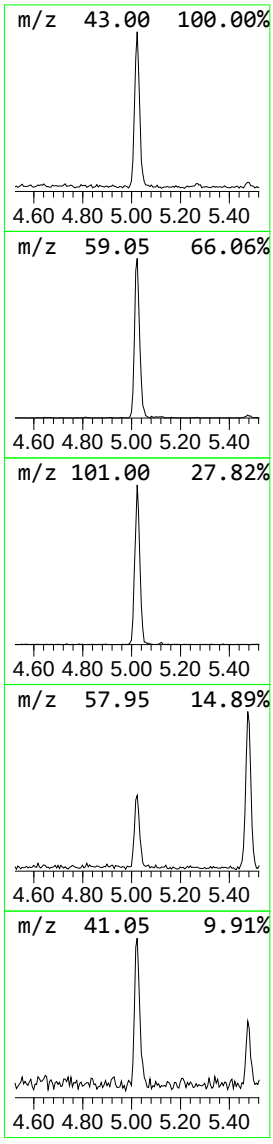
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	5.08 ng	108746	1,4-Dichlorobenzene-d4	7.905

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	35
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33
5	3-Heptadecanol	256	C17H36O	084534-30-5	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
Data File : BP019701.D
Acq On : 14 Feb 2024 14:57
Operator : MA/JU
Sample : P1453-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

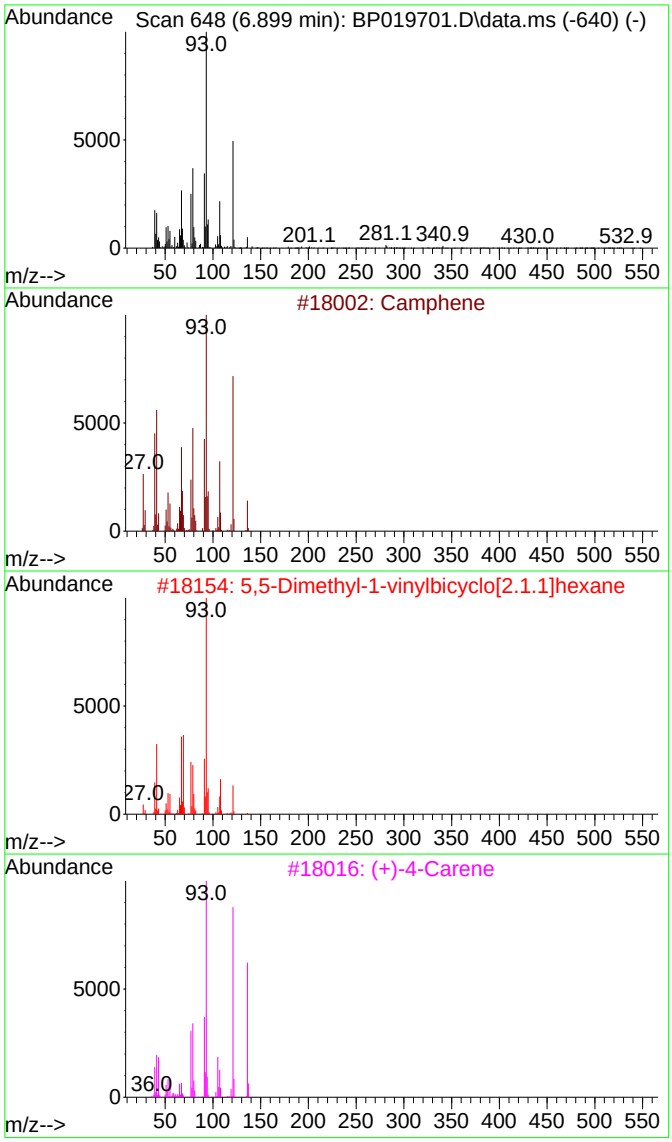
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

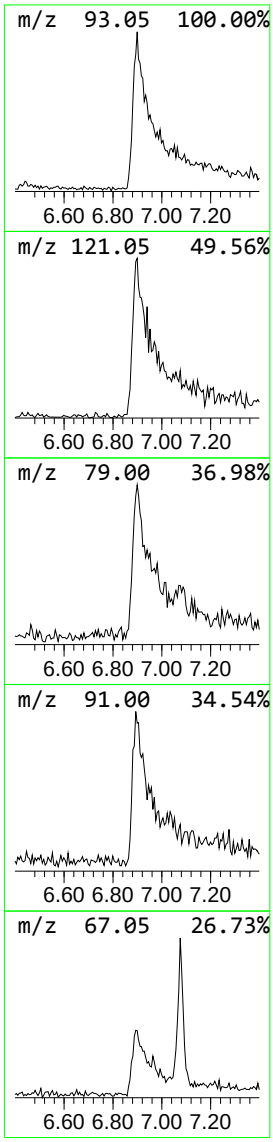
****

Peak Number 3 Camphene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.899	7.49 ng	160376	1,4-Dichlorobenzene-d4	7.905

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphene	136	C10H16	000079-92-5	76
2	5,5-Dimethyl-1-vinylbicyclo[2.1....	136	C10H16	016626-39-4	72
3	(+)-4-Carene	136	C10H16	029050-33-7	68
4	Santolina triene	136	C10H16	002153-66-4	62
5	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
Data File : BP019701.D
Acq On : 14 Feb 2024 14:57
Operator : MA/JU
Sample : P1453-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

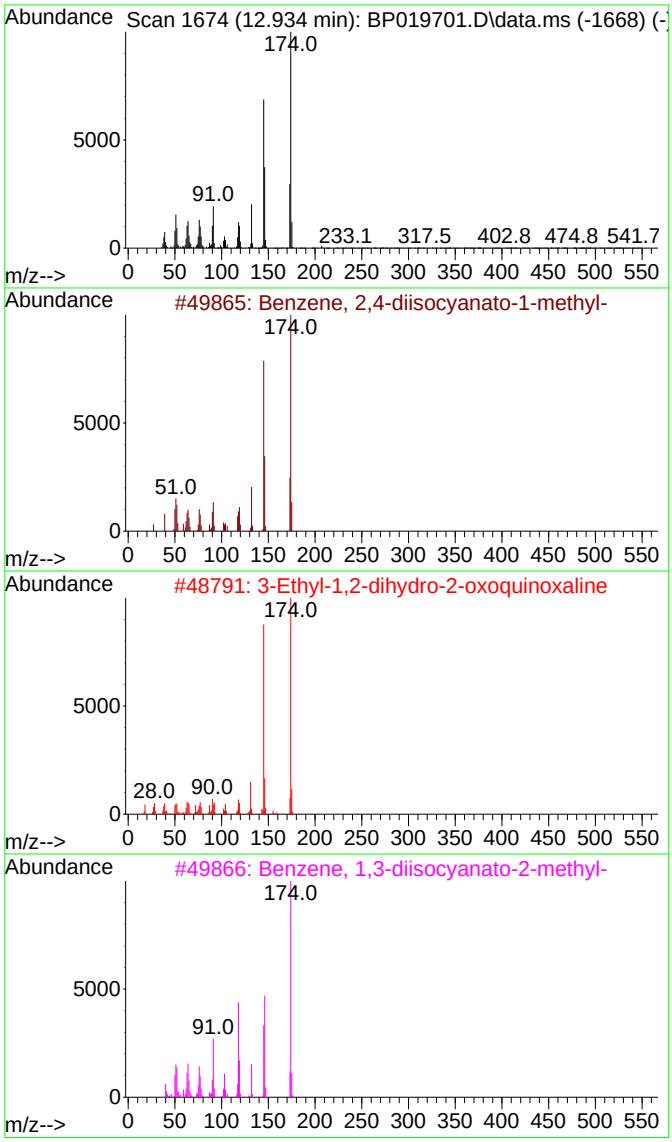
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

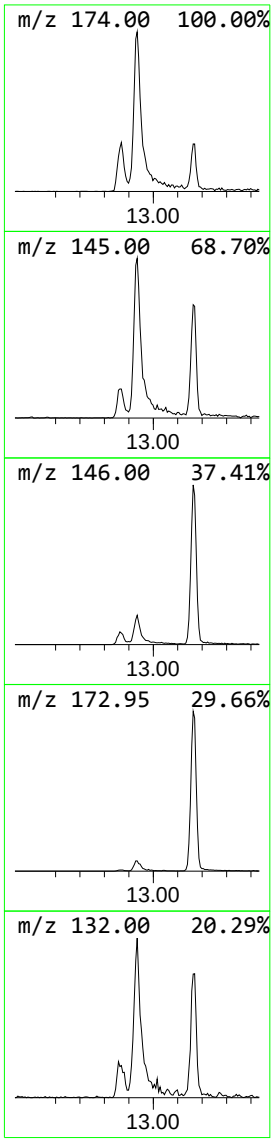
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 2,4-diisocyanato-1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.934	5.32 ng	193754	Acenaphthene-d10	14.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	97
2	3-Ethyl-1,2-dihydro-2-oxoquinoxa...	174	C10H10N2O	013297-35-3	59
3	Benzene, 1,3-diisocyanato-2-methyl-	174	C9H6N2O2	000091-08-7	58
4	5,6-Dimethyl-1H-1,3-benzodiazole...	174	C10H10N2O	920484-85-1	50
5	Juglone	174	C10H6O3	000481-39-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
Data File : BP019701.D
Acq On : 14 Feb 2024 14:57
Operator : MA/JU
Sample : P1453-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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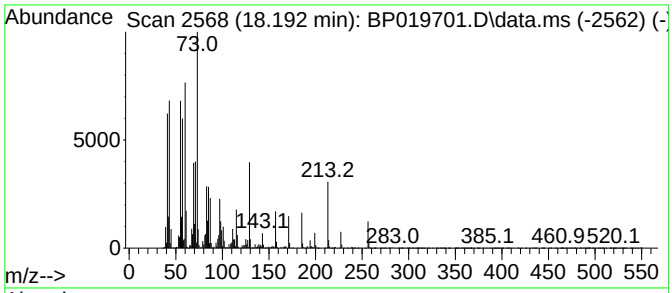
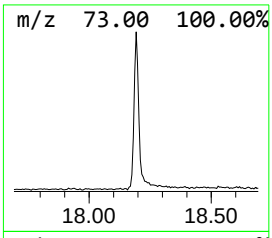
****

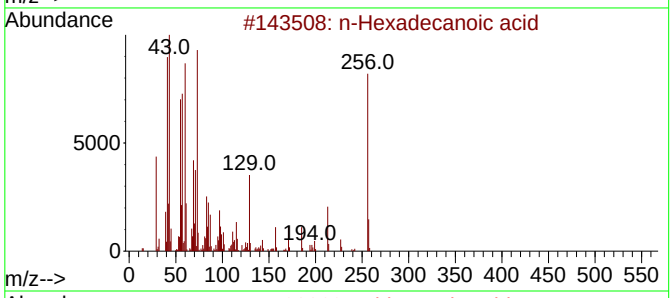
Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

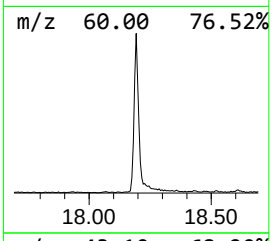
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	12.39 ng	586976	Phenanthrene-d10	17.292

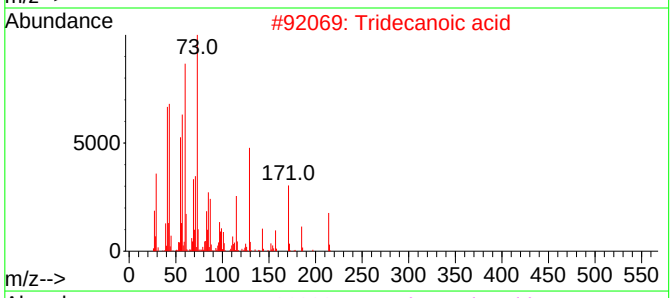
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68

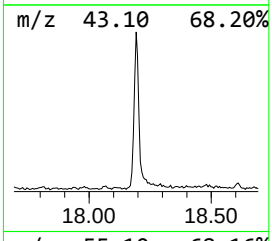


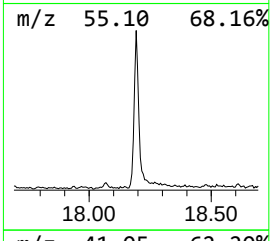


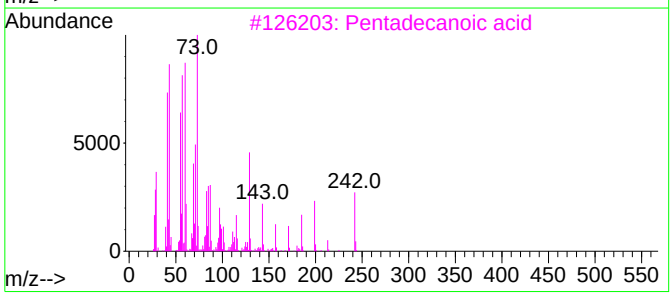


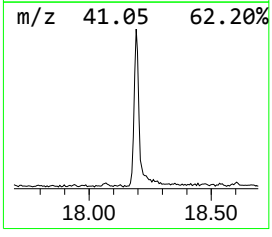












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
Data File : BP019701.D
Acq On : 14 Feb 2024 14:57
Operator : MA/JU
Sample : P1453-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

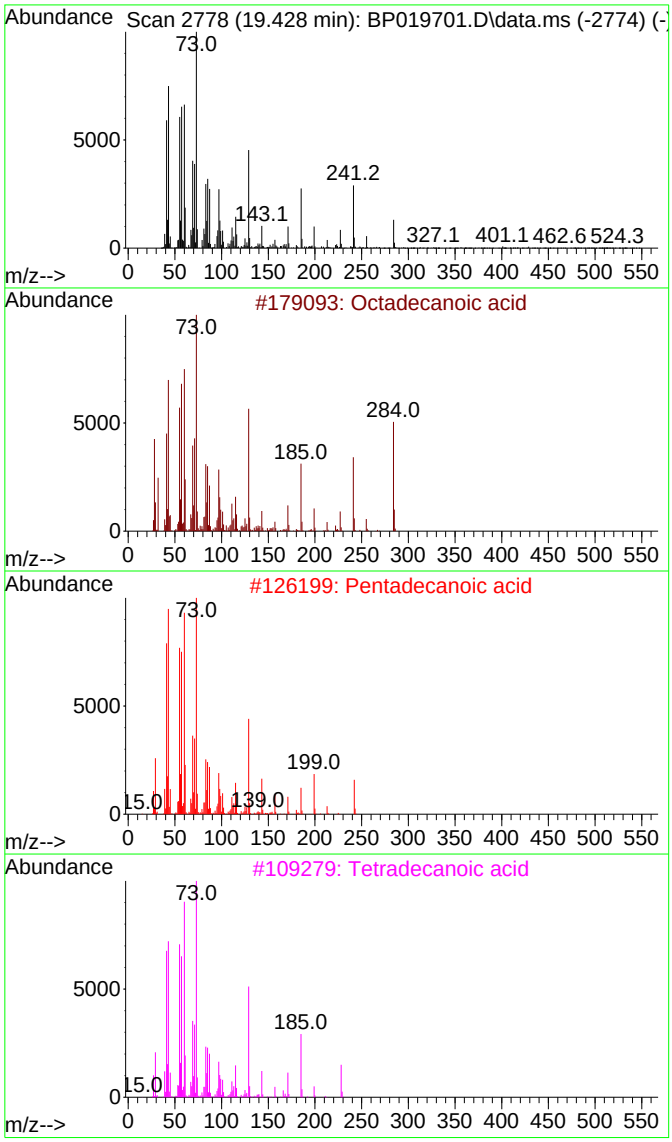
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

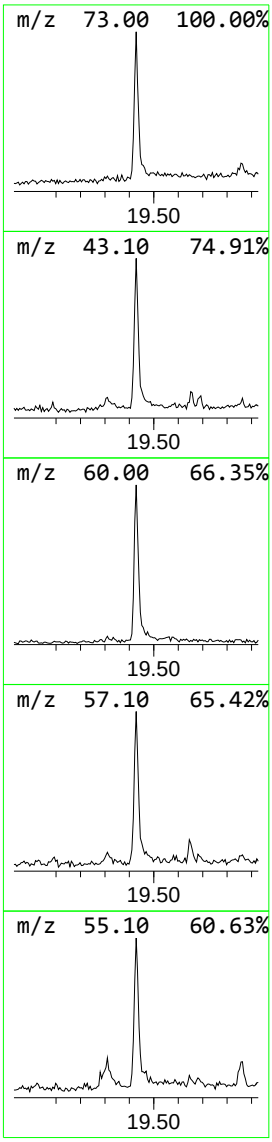
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.428	4.13 ng	237005	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	60
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Octadecane, 4-methyl-	268	C19H40	010544-95-3	25





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

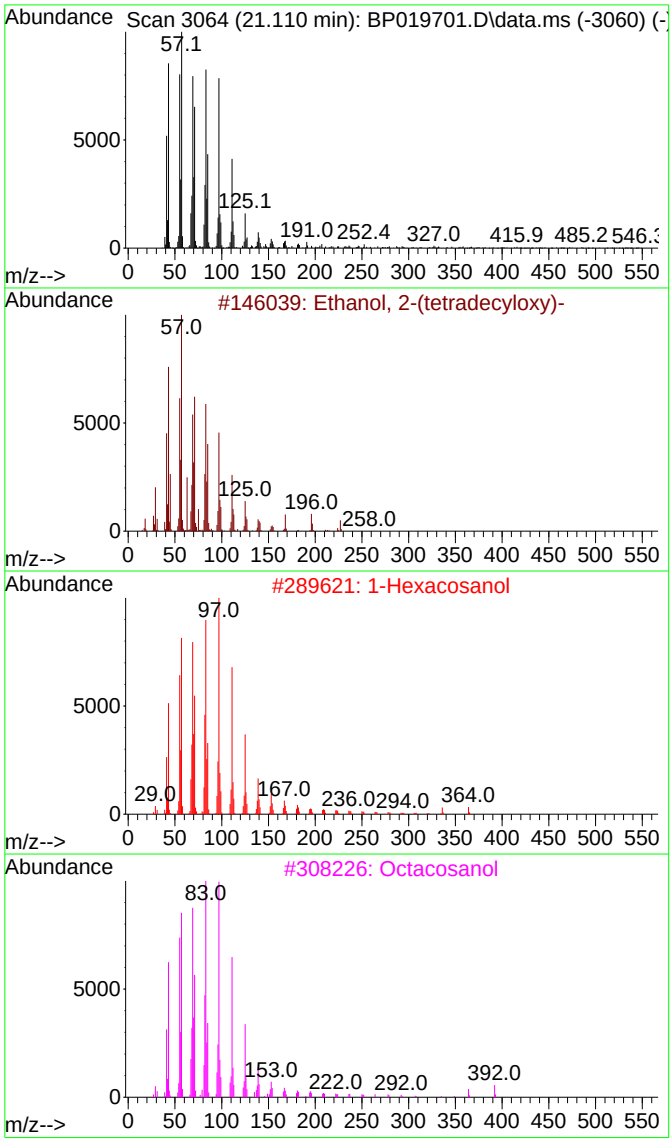
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

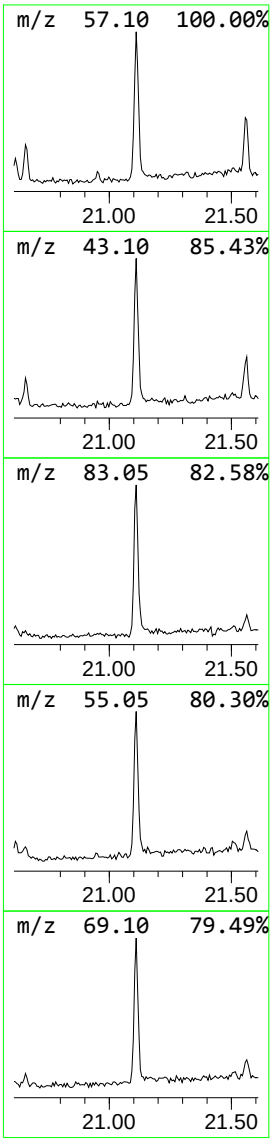
****

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.110	4.53 ng	259721	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	1-Hexacosanol	382	C26H54O	000506-52-5	90
3	Octacosanol	410	C28H58O	000557-61-9	90
4	1-Hexacosene	364	C26H52	018835-33-1	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021424\
Data File : BP019701.D
Acq On : 14 Feb 2024 14:57
Operator : MA/JU
Sample : P1453-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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
R-(-)-1,2-propa...	3.628	2.6	ng	55110	1	7.905	428234	20.0
2-Pentanone, 4-...	5.022	5.1	ng	108746	1	7.905	428234	20.0
Camphene	6.899	7.5	ng	160376	1	7.905	428234	20.0
Benzene, 2,4-di...	12.934	5.3	ng	193754	3	14.540	728772	20.0
n-Hexadecanoic ...	18.192	12.4	ng	586976	4	17.292	947853	20.0
Octadecanoic acid	19.428	4.1	ng	237005	5	21.386	1146770	20.0
Ethanol, 2-(tet...	21.110	4.5	ng	259721	5	21.386	1146770	20.0