LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002328.D
Acq On : 29 May 2020 22:35
Operator : CG/JU
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM81-COMP-2020-0-6

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\8270-BP052720.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.222	391	397	412	rBV	3217190	4879827	48.37%	5.421%
2	6.793	656	664	675	rBV	3487712	5527244	54.79%	6.141%
3	7.605	795	802	813	rBV	1557680	2448979	24.28%	2.721%
4	7.922	849	856	865	rBV	2994132	4845270	48.03%	5.383%
5	8.746	984	996	1011	rBV	2329233	3907792	38.74%	4.342%
6	10.381	1266	1274	1281	rBV	2035692	3478464	34.48%	3.865%
7	12.257	1587	1593	1601	rVB2	190072	307431	3.05%	0.342%
8	12.869	1690	1697	1714	rBV	5568473	8297325	82.25%	9.218%
9	13.175	1742	1749	1757	rBV	1024328	1554462	15.41%	1.727%
10	13.710	1832	1840	1850	rBV	276063	410592	4.07%	0.456%
11	14.251	1925	1932	1939	rBV2	2980576	4398378	43.60%	4.887%
12	15.416	2124	2130	2136	rBV	385357	506581	5.02%	0.563%
13	15.745	2179	2186	2196	rBV	3687585	5565888	55.17%	6.184%
14	17.010	2395	2401	2405	rBV	3528665	4938356	48.95%	5.486%
15	17.051	2405	2408	2413	rVB	634617	836714	8.29%	0.930%
16	17.139	2419	2423	2429	rVB	207731	276135	2.74%	0.307%
17	17.416	2465	2470	2476	rBV	55241	110451	1.09%	0.123%
18	17.881	2544	2549	2554	rBV2	163674	257242	2.55%	0.286%
19	17.939	2554	2559	2566	rVV2	310251	478694	4.75%	0.532%
20	18.069	2577	2581	2586	rBV2	145890	243759	2.42%	0.271%
21	18.775	2697	2701	2707	rBV2	168140	256082	2.54%	0.285%
22	18.910	2721	2724	2733	rVB4	59727	117961	1.17%	0.131%
23	19.033	2740	2745	2750	rVB	1350342	1731218	17.16%	1.923%
24	19.086	2751	2754	2760	rVV2	178475	208099	2.06%	0.231%
25	19.386	2796	2805	2809	rBV	1196346	1932329	19.15%	2.147%
26	19.598	2836	2841	2852	rVB	7924500	10088040	100.00%	11.208%
27	19.875	2885	2888	2894	rVB	174030	258135	2.56%	0.287%
28	19.969	2901	2904	2909	rBV	136577	171198	1.70%	0.190%
29	20.028	2910	2914	2918	rVB2	122468	156488	1.55%	0.174%
30	20.833	3048	3051	3052	rBV	230232	200325	1.99%	0.223%
31	20.857	3052	3055	3059	rVB	588688	647857	6.42%	0.720%
32	21.110	3092	3098	3102	rBV2	4091783	6145264	60.92%	6.827%
33	21.145	3102	3104	3111	rVB	655088	796351	7.89%	0.885%
34	21.733	3201	3204	3210	rVB2	311768	416431	4.13%	0.463%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002328.D
Acq On : 29 May 2020 22:35
Operator : CG/JU
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM81-COMP-2020-0-6

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\8270-BP052720.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.416	3317	3320	3331	rVB	257144	361827	3.59%	0.402%
36	22.657	3357	3361	3365	rBV	544351	1094670	10.85%	1.216%
37	22.704	3365	3369	3372	rVV2	844021	1343713	13.32%	1.493%
38	22.739	3372	3375	3385	rVB3	565268	864270	8.57%	0.960%
39	23.127	3437	3441	3450	rVB	385077	705220	6.99%	0.783%
40	23.221	3452	3457	3462	rBV	482975	875000	8.67%	0.972%
41	23.321	3468	3474	3480	rVB	2489875	4442260	44.03%	4.935%
42	23.921	3571	3576	3583	rVB	759772	1356773	13.45%	1.507%
43	23.998	3585	3589	3598	rVB	352009	650510	6.45%	0.723%
44	25.545	3846	3852	3865	rVB4	661855	1919671	19.03%	2.133%

Sum of corrected areas: 90009276

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
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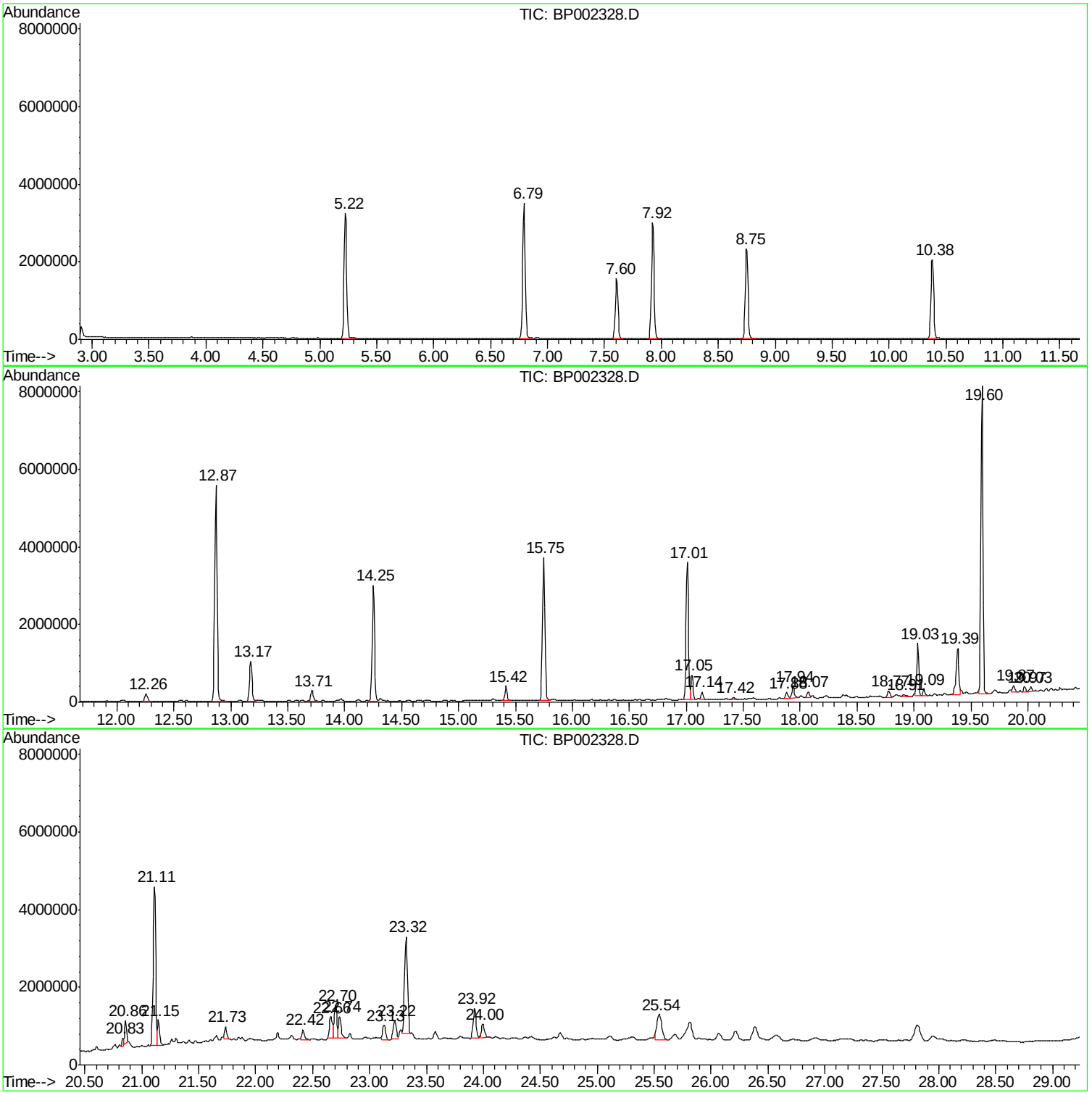
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NM81-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002328.D
Acq On : 29 May 2020 22:35
Operator : CG/JU
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM81-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

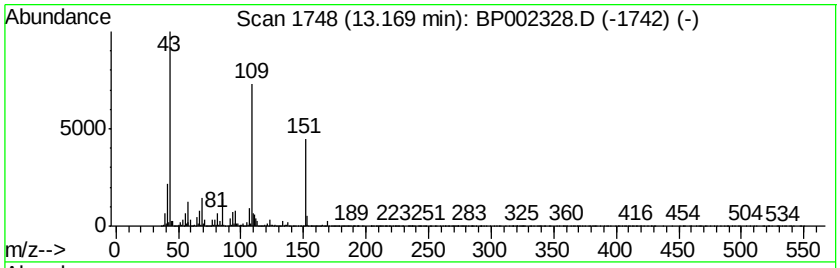
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

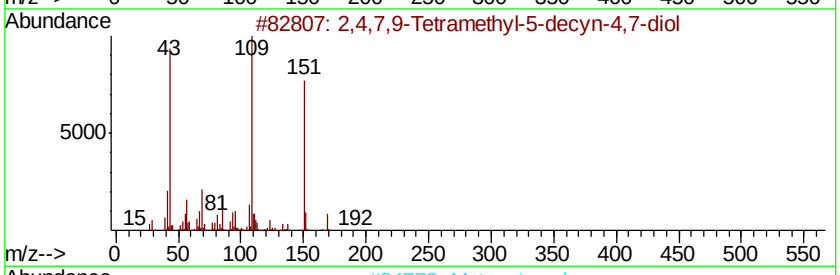
****

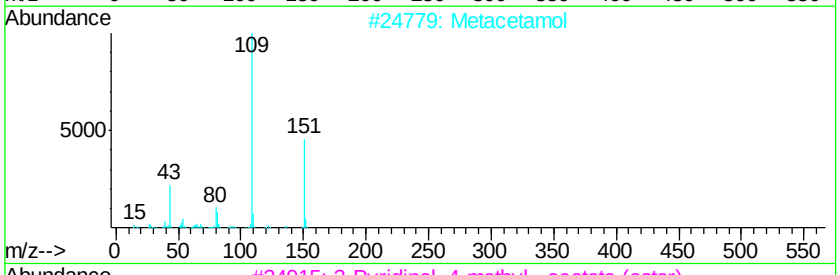
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

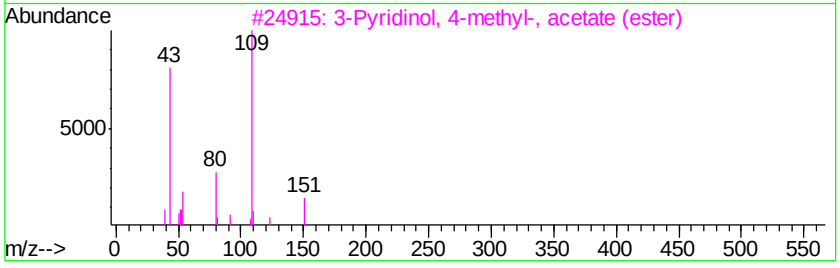
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	7.07 ng	1554460	Acenaphthene-d10	14.25

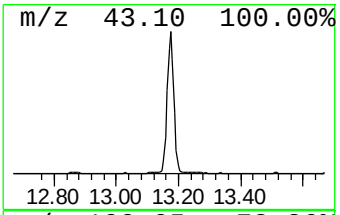
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	59
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
5	Acetaminophen	151	C8H9NO2	000103-90-2	59

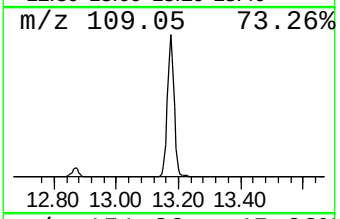


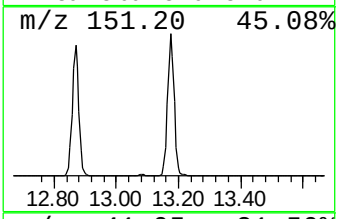


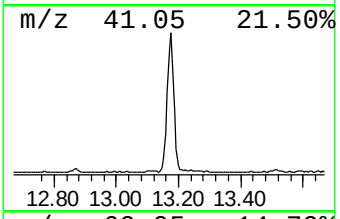


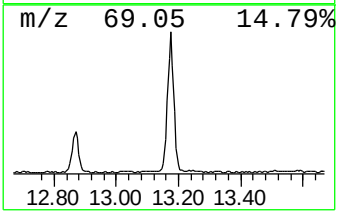












Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002328.D
Acq On : 29 May 2020 22:35
Operator : CG/JU
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM81-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

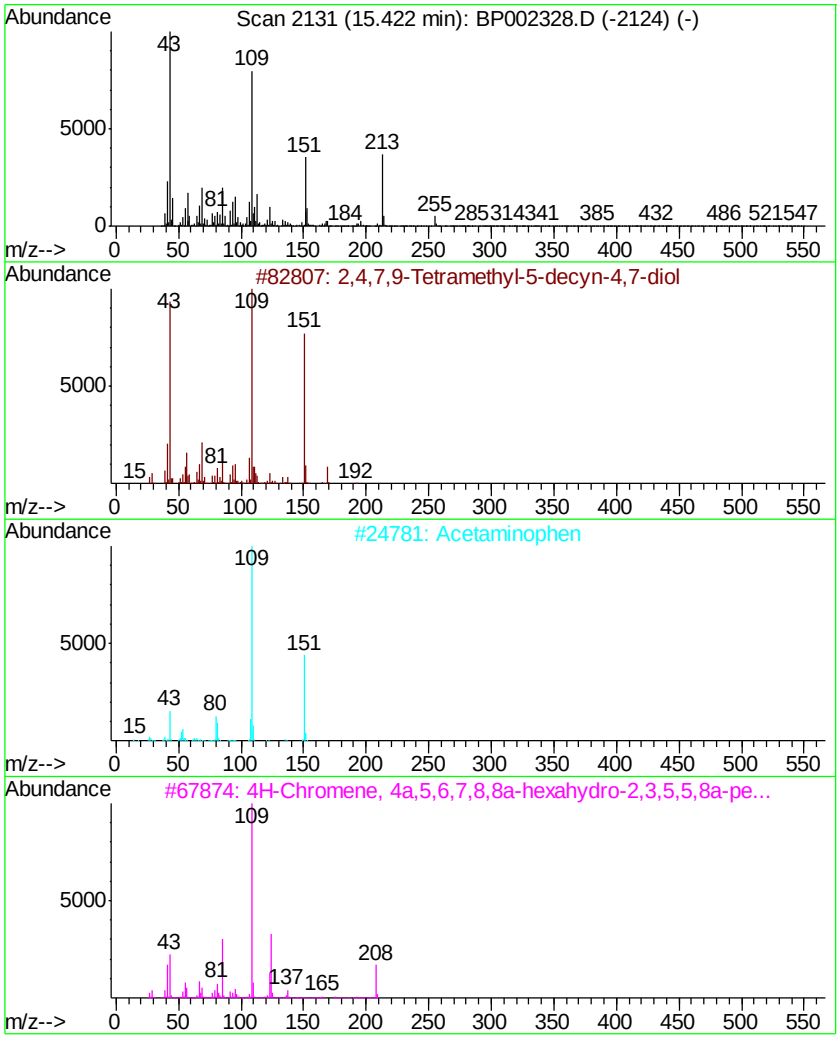
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

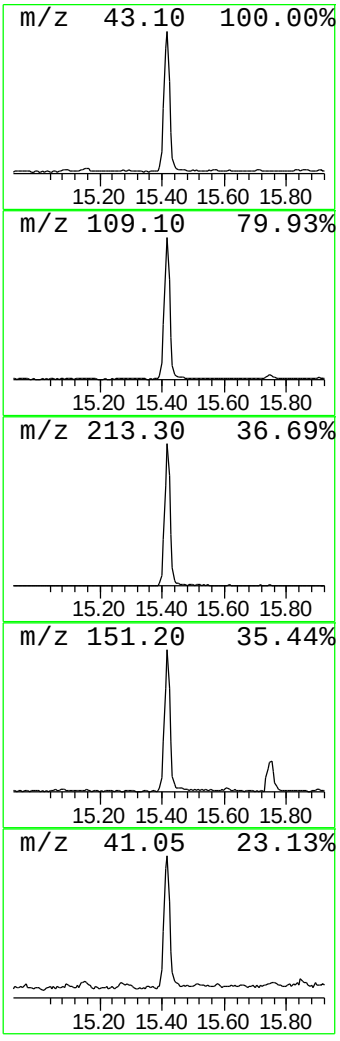
****

Peak Number 3 unknown15.42 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	2.30 ng	506581	Acenaphthene-d10	14.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	59
2	Acetaminophen	151	C8H9NO2	000103-90-2	46
3	4H-Chromene, 4a,5,6,7,8,8a-hexah...	208	C14H24O	1000196-77-4	43
4	Metacetamol	151	C8H9NO2	000621-42-1	43
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002328.D
Acq On : 29 May 2020 22:35
Operator : CG/JU
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM81-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

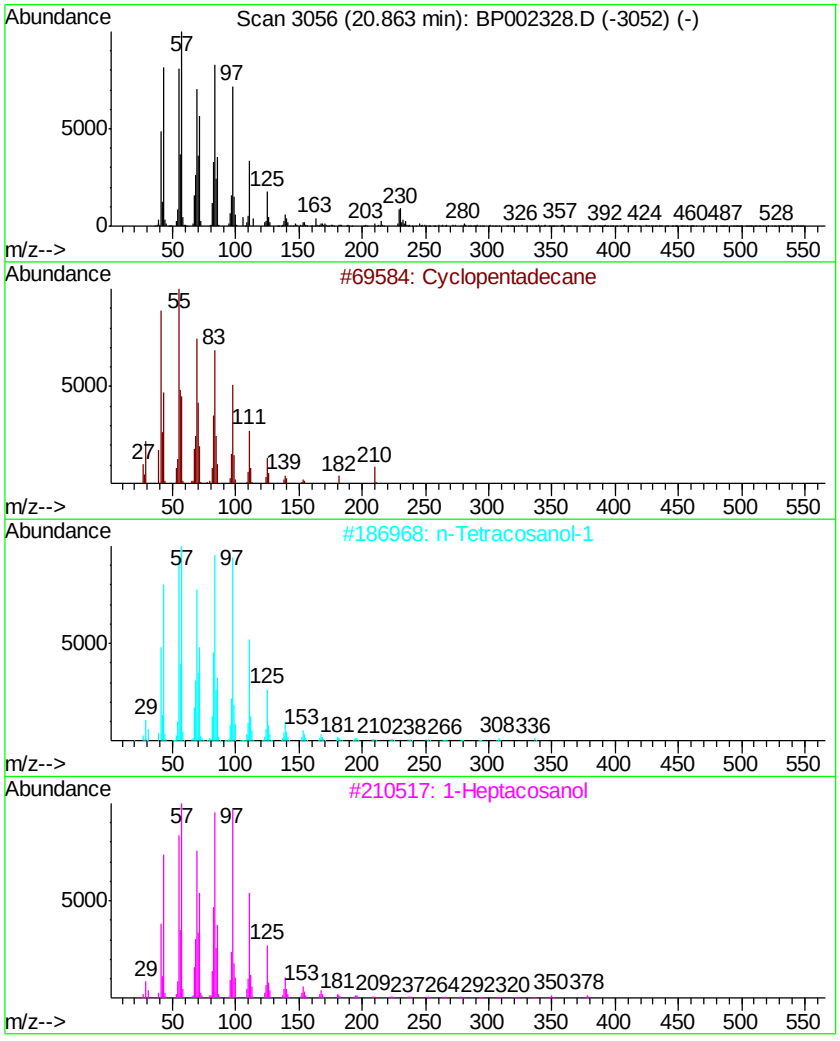
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

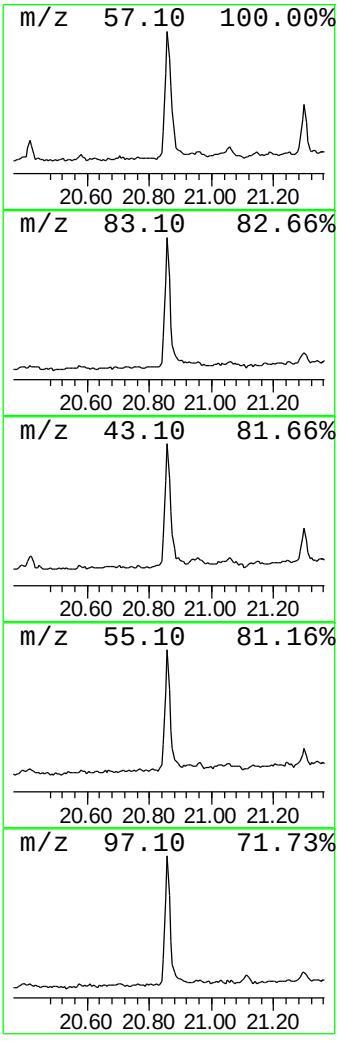
****

Peak Number 4 Cyclopentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	2.11 ng	647857	Chrysene-d12	21.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002328.D
Acq On : 29 May 2020 22:35
Operator : CG/JU
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM81-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

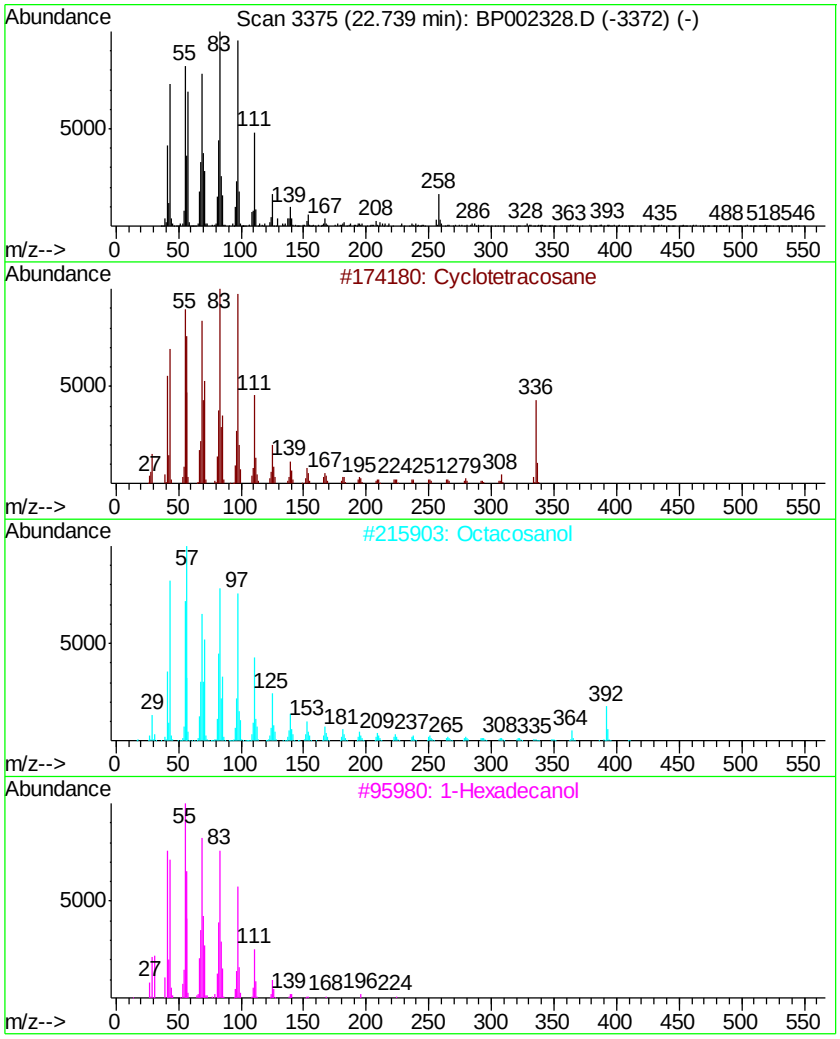
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

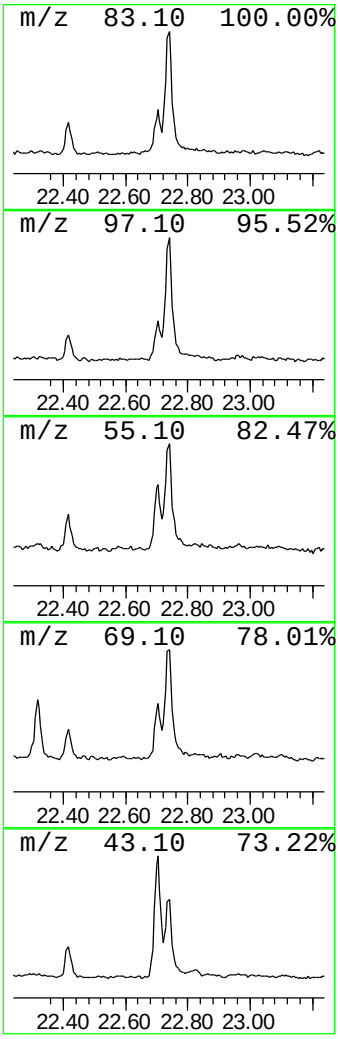
****

Peak Number 5 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.74	3.89 ng	864270	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	93
2	Octacosanol	410	C28H58O	000557-61-9	89
3	1-Hexadecanol	242	C16H34O	036653-82-4	58
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	58
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002328.D
Acq On : 29 May 2020 22:35
Operator : CG/JU
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM81-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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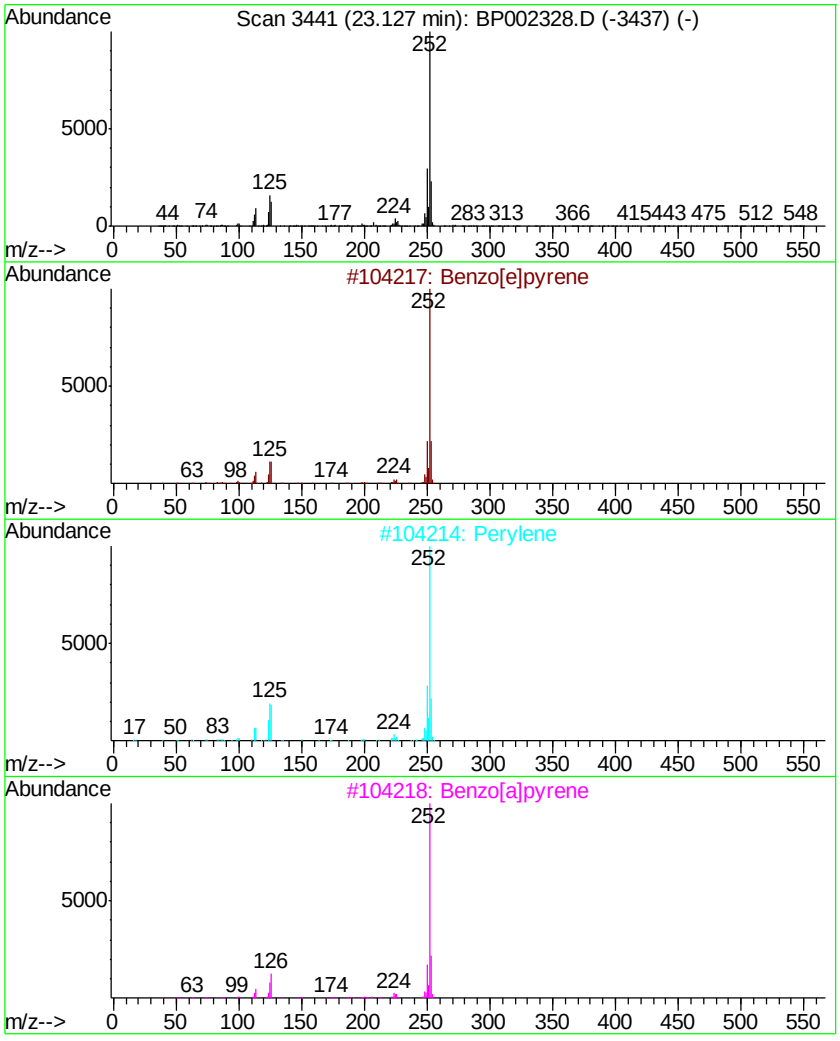
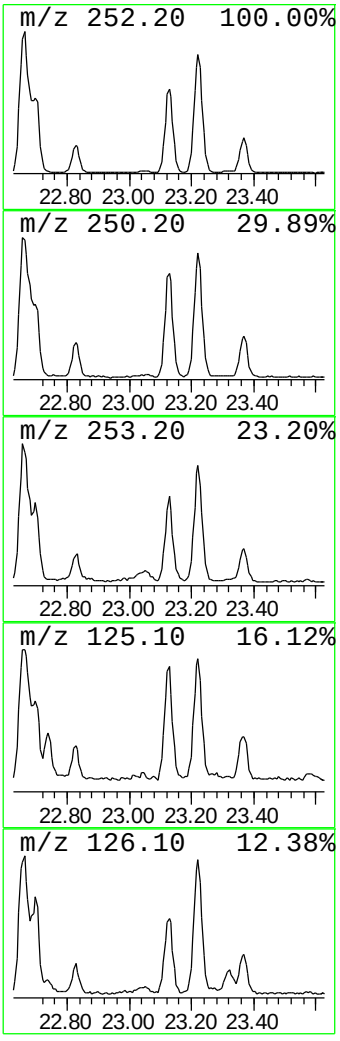
Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.13	3.18 ng	705220	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	98
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002328.D
Acq On : 29 May 2020 22:35
Operator : CG/JU
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM81-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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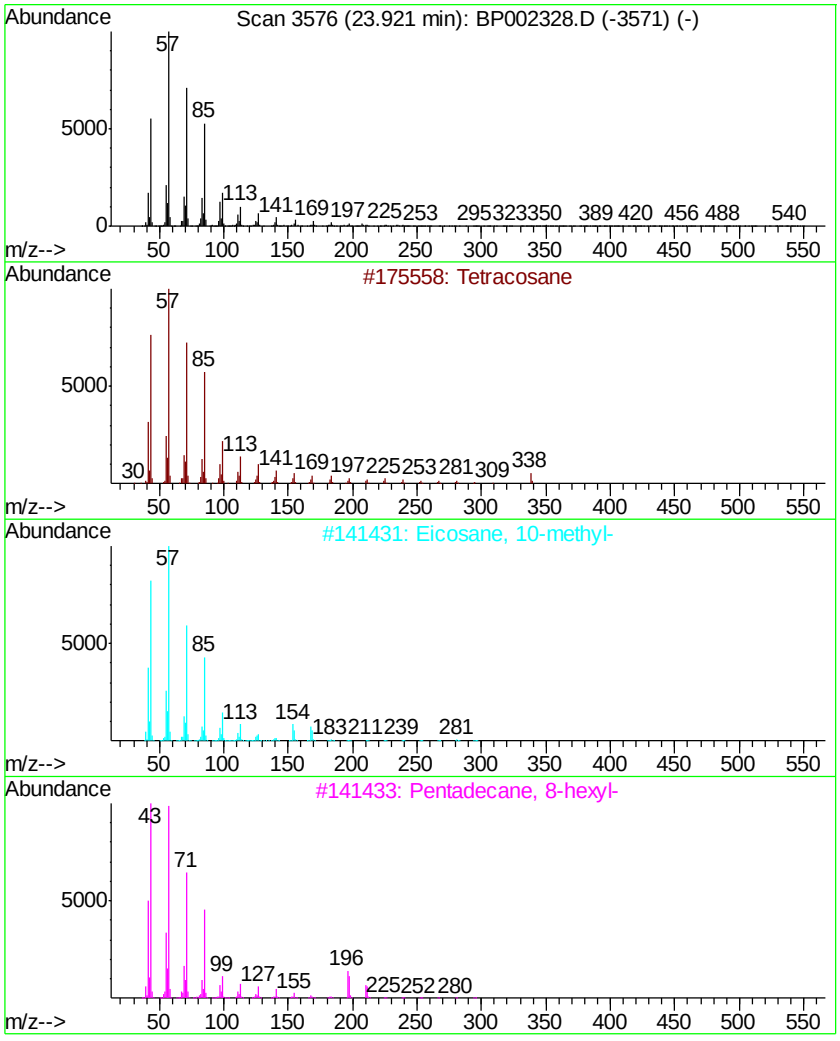
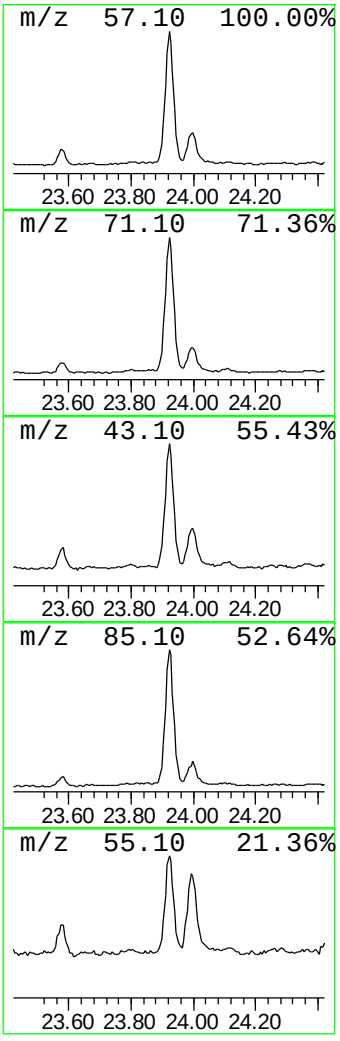
Peak Number 7 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	6.11 ng	1356770	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Octacosane	394	C28H58	000630-02-4	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002328.D
Acq On : 29 May 2020 22:35
Operator : CG/JU
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM81-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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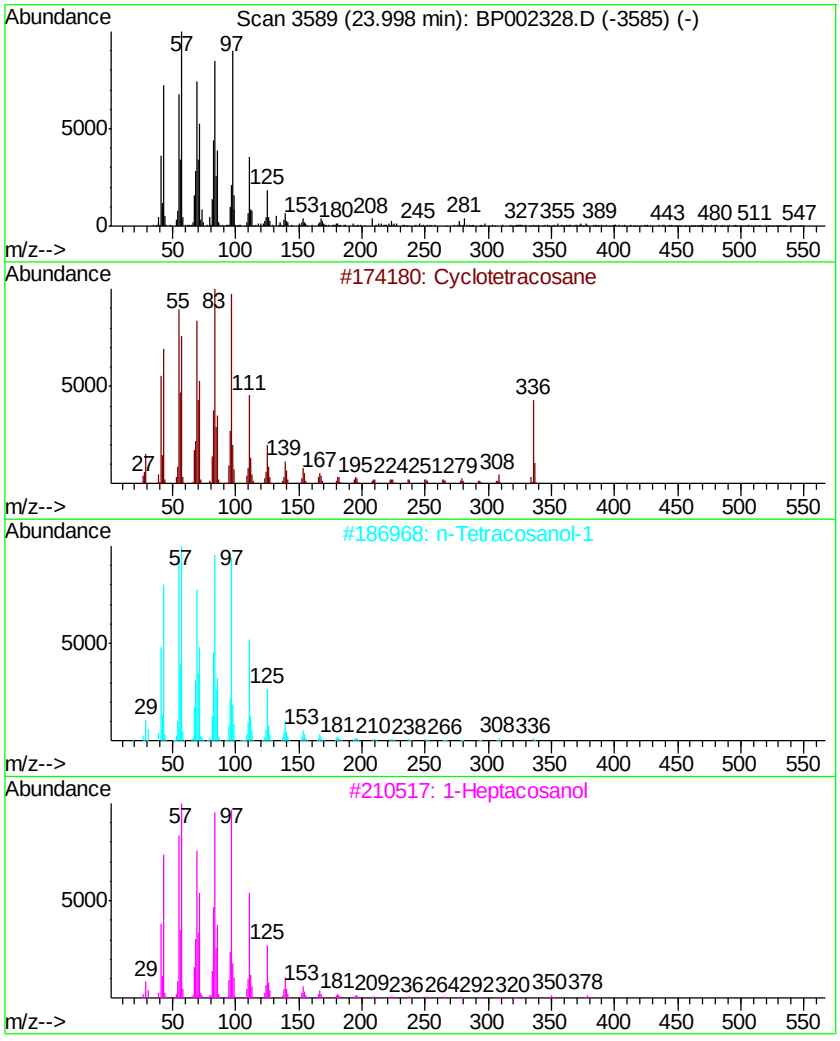
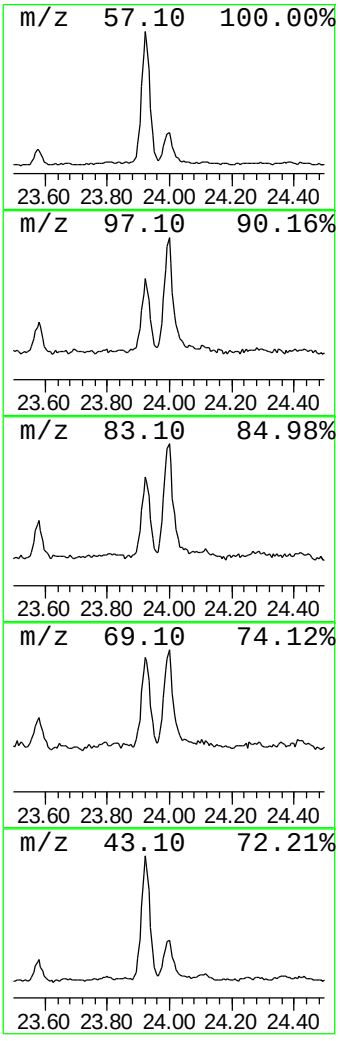
Peak Number 8 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	2.93 ng	650510	Perylene-d12	23.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP052920\
Data File : BP002328.D
Acq On : 29 May 2020 22:35
Operator : CG/JU
Sample : L2745-04 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : NM81-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2,4,7,9-Tetrameth...	13.17	7.1	ng	1554460	3	14.25	4398380	20.0
unknown15.42	15.42	2.3	ng	506581	3	14.25	4398380	20.0
Cyclopentadecane	20.86	2.1	ng	647857	5	21.11	6145260	20.0
Cyclotetracosane	22.74	3.9	ng	864270	6	23.32	4442260	20.0
Benzo[e]pyrene	23.13	3.2	ng	705220	6	23.32	4442260	20.0
Tetracosane	23.92	6.1	ng	1356770	6	23.32	4442260	20.0
n-Tetracosanol-1	24.00	2.9	ng	650510	6	23.32	4442260	20.0