LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122619\
Data File : BP001422.D
Acq On : 26 Dec 2019 15:26
Operator : JU
Sample : PB125704BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB125704BL

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-BP121919.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	5.593	592	596	611	rVB	80681	125830	6.40%	1.101%
2	6.205	694	700	715	rBV	543163	690276	35.13%	6.041%
3	7.740	956	961	974	rBV	358350	457665	23.29%	4.005%
4	7.928	987	993	1006	rBV	1048928	1241371	63.18%	10.864%
5	8.281	1048	1053	1061	rBV	194363	227792	11.59%	1.994%
6	8.528	1088	1095	1104	rBV	821672	974138	49.58%	8.525%
7	9.169	1196	1204	1208	rBV	649430	826970	42.09%	7.237%
8	10.316	1391	1399	1411	rBV	207129	270201	13.75%	2.365%
9	12.098	1695	1702	1721	rBV	1230039	1531861	77.97%	13.406%
10	13.181	1878	1886	1901	rBV	252918	328902	16.74%	2.878%
11	14.475	2100	2106	2137	rBV	821273	1123914	57.21%	9.836%
12	15.580	2288	2294	2305	rBV	294570	366125	18.64%	3.204%
13	15.722	2313	2318	2333	rVB2	35536	49499	2.52%	0.433%
14	17.869	2676	2683	2686	rBV	1848702	1964706	100.00%	17.194%
15	19.221	2908	2913	2918	rBV	306286	332389	16.92%	2.909%
16	19.904	3024	3029	3039	rBV	38207	46222	2.35%	0.405%
17	20.274	3088	3092	3099	rBV	76292	91289	4.65%	0.799%
18	20.668	3154	3159	3169	rBV	101784	132154	6.73%	1.157%
19	20.992	3208	3214	3225	rVB	203296	297099	15.12%	2.600%
20	21.104	3227	3233	3241	rBV	102394	148435	7.56%	1.299%
21	21.592	3310	3316	3323	rBV	67653	112767	5.74%	0.987%
22	22.157	3405	3412	3421	rBV2	31935	62444	3.18%	0.546%
23	22.815	3517	3524	3531	rVB4	10271	24477	1.25%	0.214%

Sum of corrected areas: 11426526

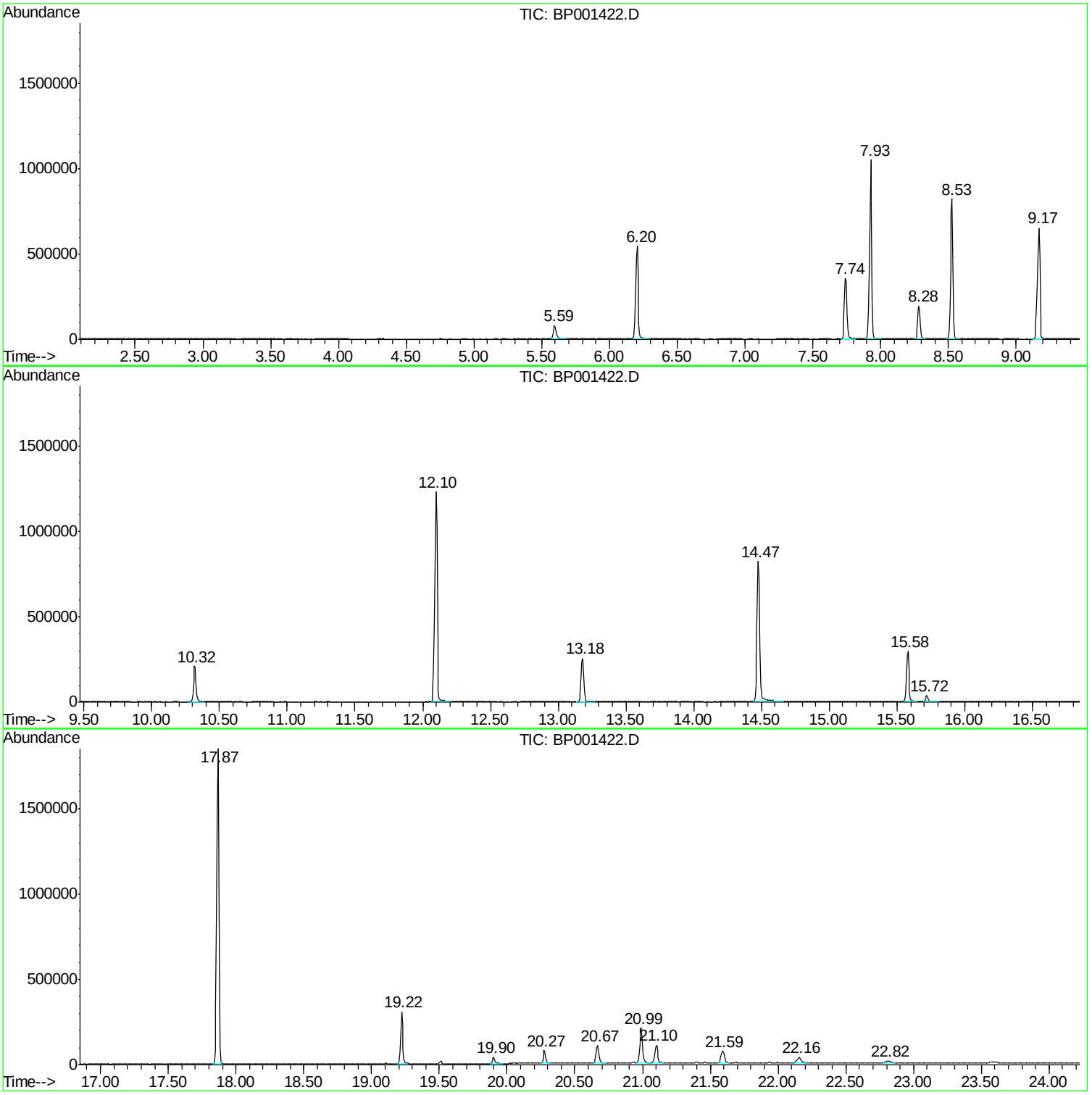
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122619\
Data File : BP001422.D
Acq On : 26 Dec 2019 15:26
Operator : JU
Sample : PB125704BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB125704BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122619\
Data File : BP001422.D
Acq On : 26 Dec 2019 15:26
Operator : JU
Sample : PB125704BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB125704BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

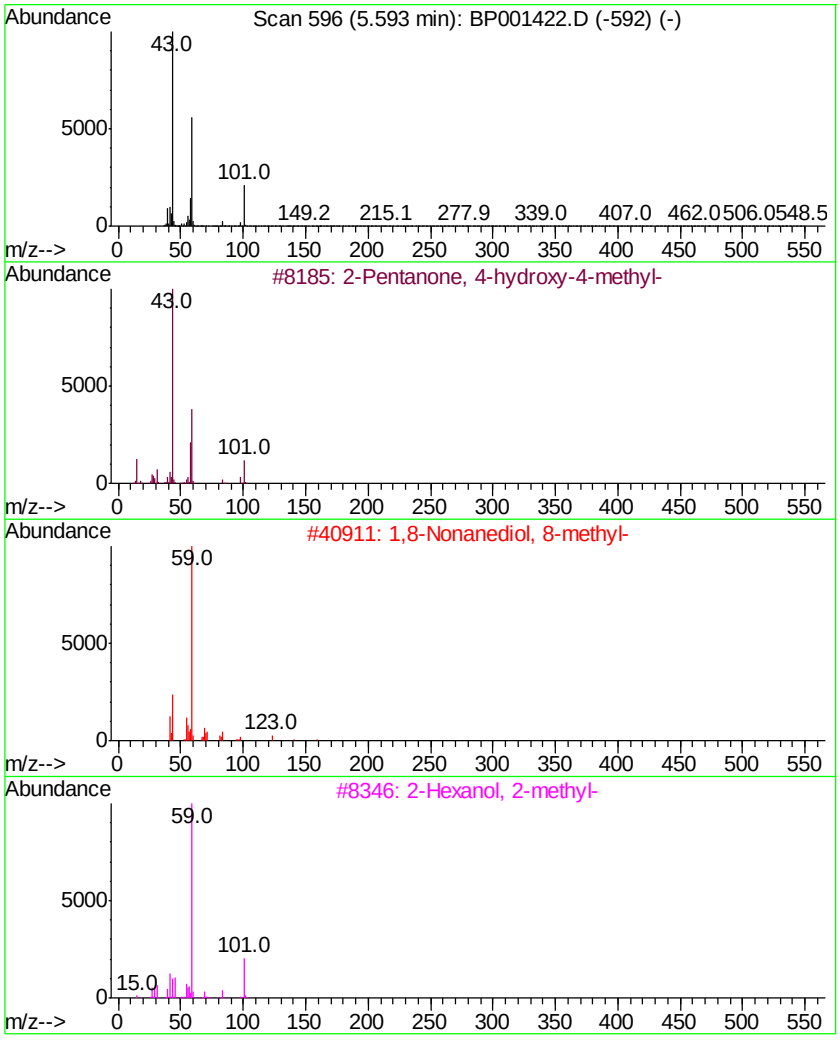
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

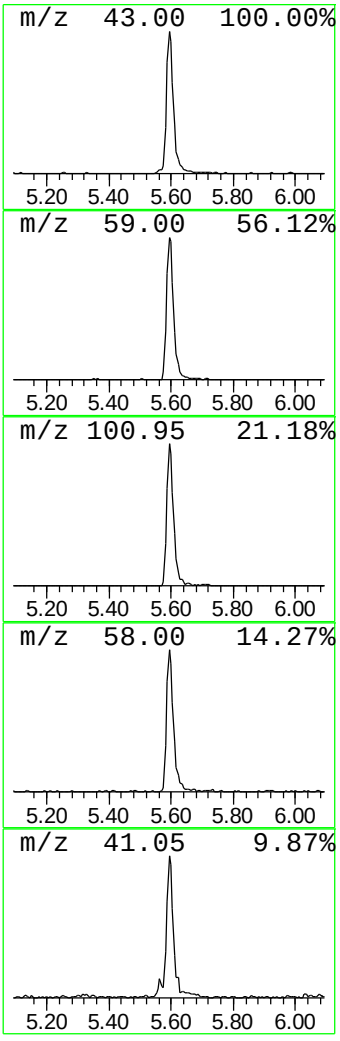
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	11.05 ng	125830	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	32
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122619\
Data File : BP001422.D
Acq On : 26 Dec 2019 15:26
Operator : JU
Sample : PB125704BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB125704BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

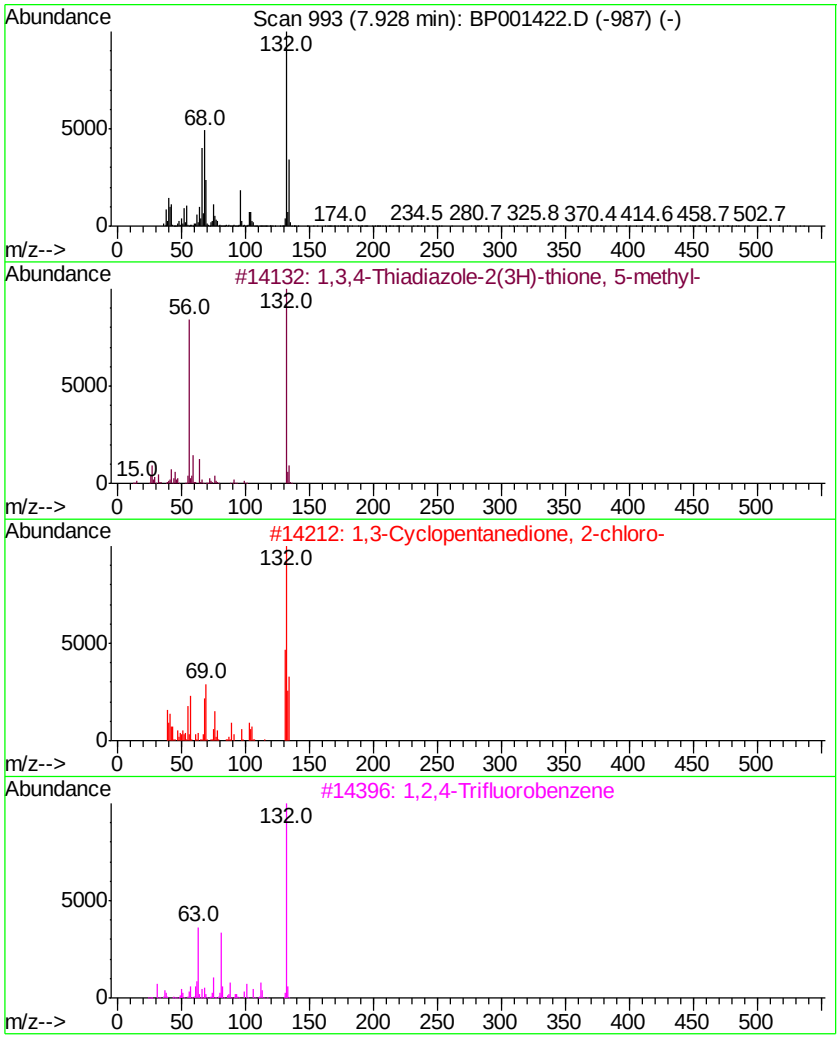
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

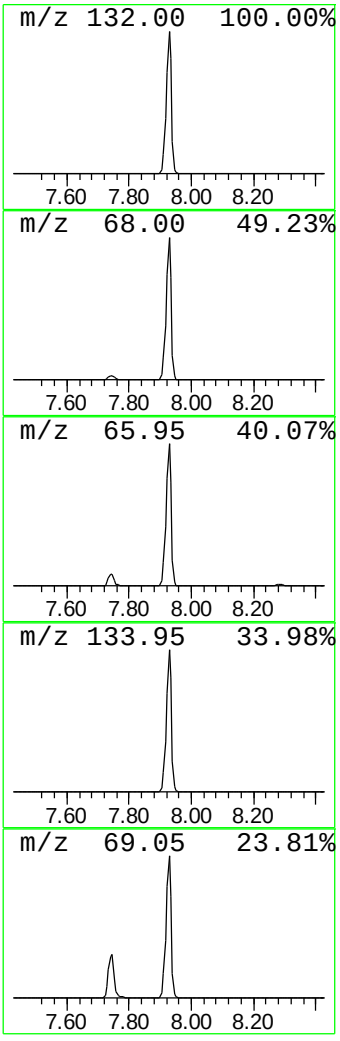
****

Peak Number 2 unknown7.93 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	108.99 ng	1241370	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
3	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122619\
Data File : BP001422.D
Acq On : 26 Dec 2019 15:26
Operator : JU
Sample : PB125704BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB125704BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

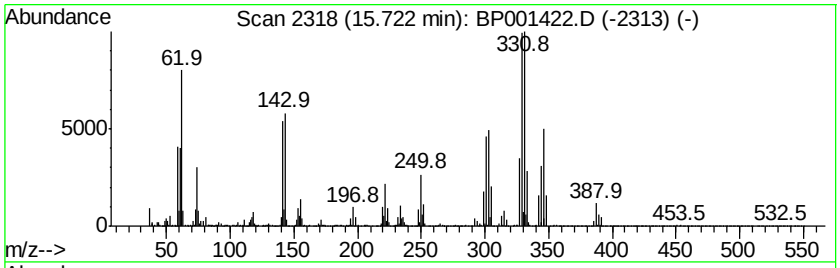
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

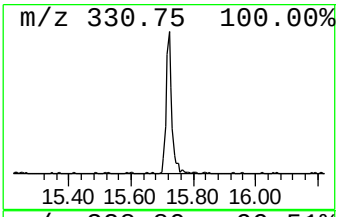
****

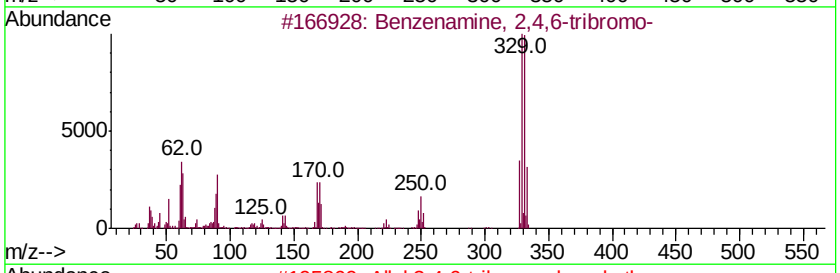
Peak Number 4 Benzenamine, 2,4,6-tribromo- Concentration Rank 10

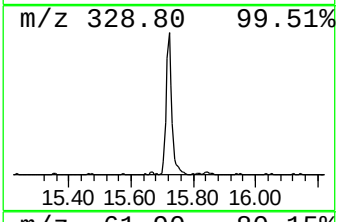
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.70 ng	49499	Phenanthrene-d10	15.58

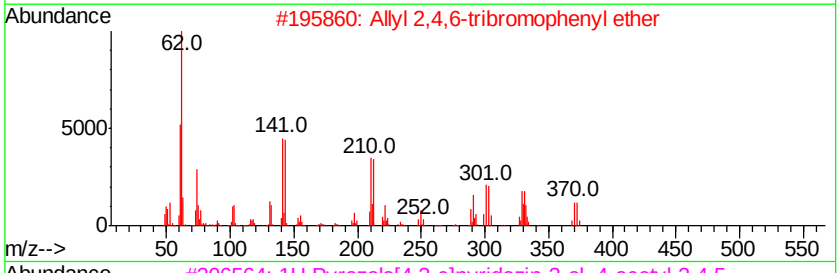
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	55
2	Allyl 2,4,6-tribromophenyl ether	368	C9H7Br3O	003278-89-5	43
3	1H-Pyrazolo[4,3-c]pyridazin-3-ol...	388	C22H20N4O3	035426-81-4	17
4	Tellurium, bis[(.eta.-5-cyclopen...	612	C22H40Ni2P2Te	1000161-69-8	17
5	Triethylphosphine	118	C6H15P	000554-70-1	17

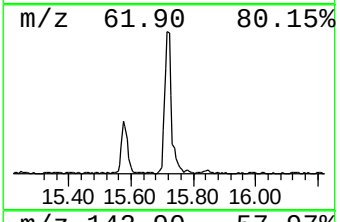


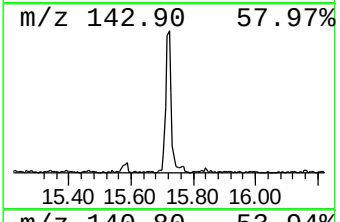


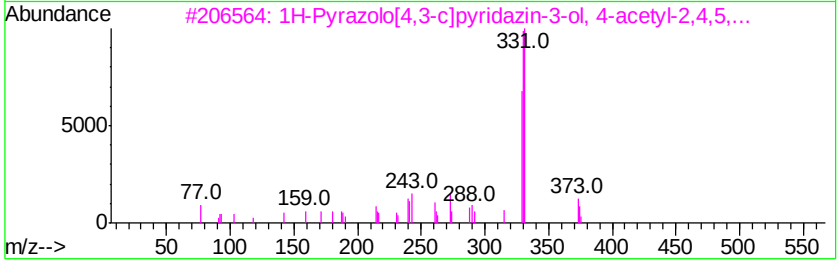


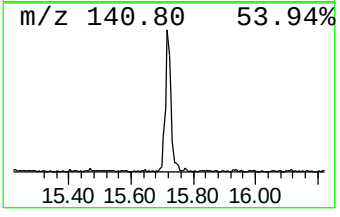












Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122619\
Data File : BP001422.D
Acq On : 26 Dec 2019 15:26
Operator : JU
Sample : PB125704BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB125704BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

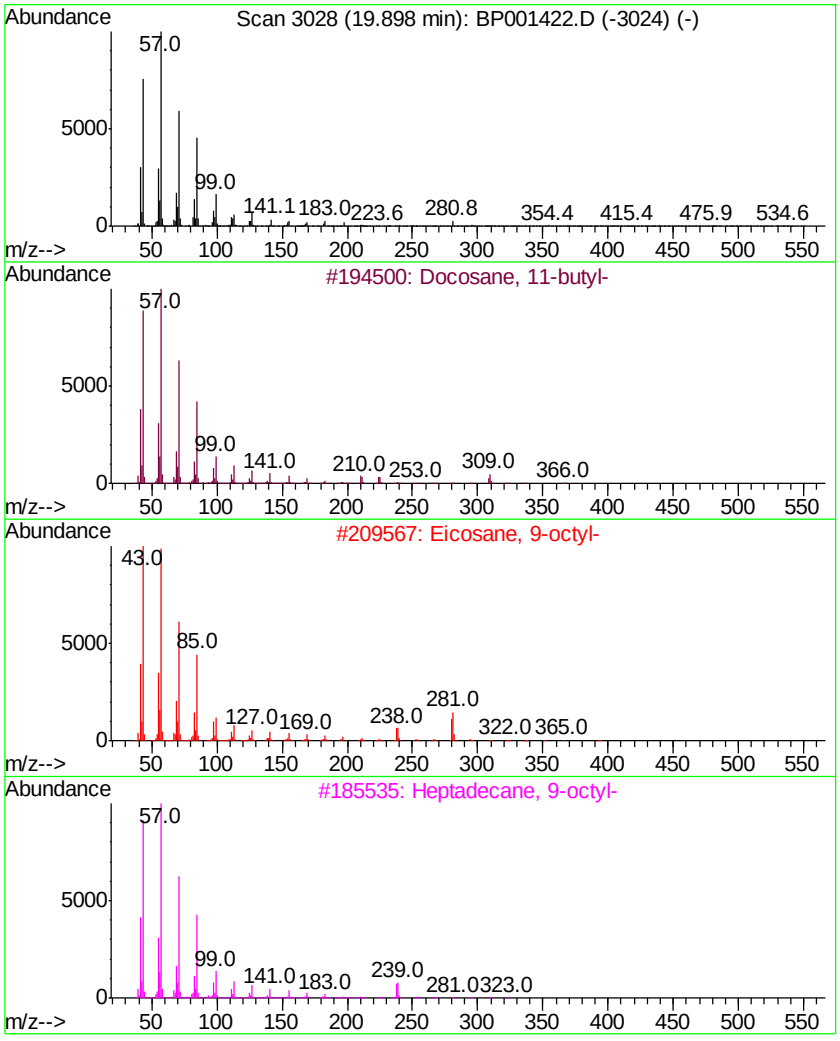
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

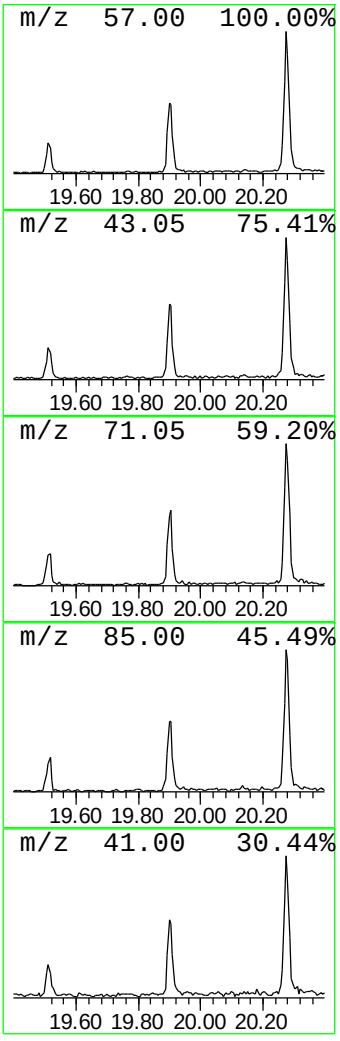
****

Peak Number 5 Docosane, 11-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	2.78 ng	46222	Chrysene-d12	19.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	98
2	Eicosane, 9-octyl-	394	C28H58	013475-77-9	95
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	94
5	Heptacosane	380	C27H56	000593-49-7	91





Library Search Compound Report

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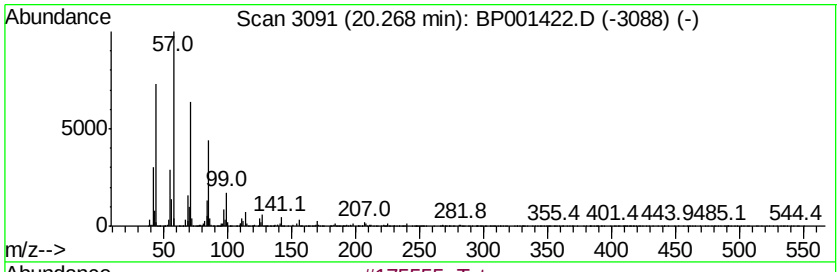
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

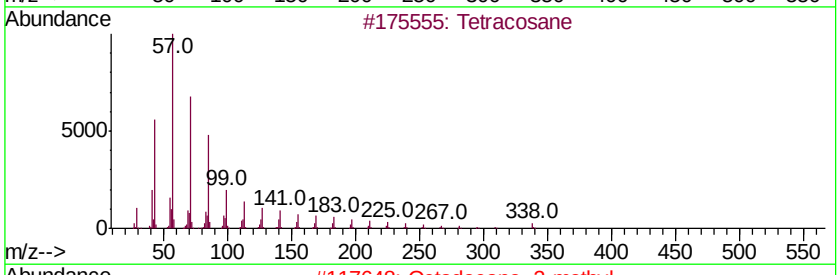
****

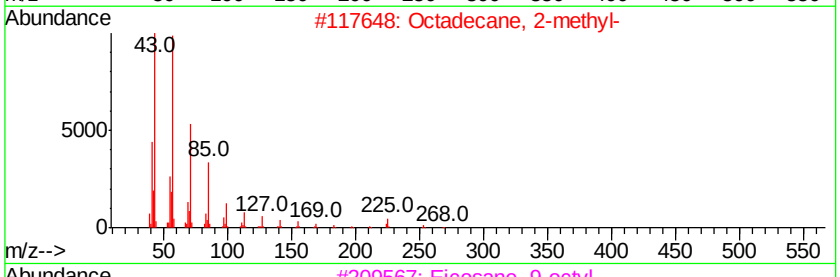
Peak Number 6 Tetracosane Concentration Rank 7

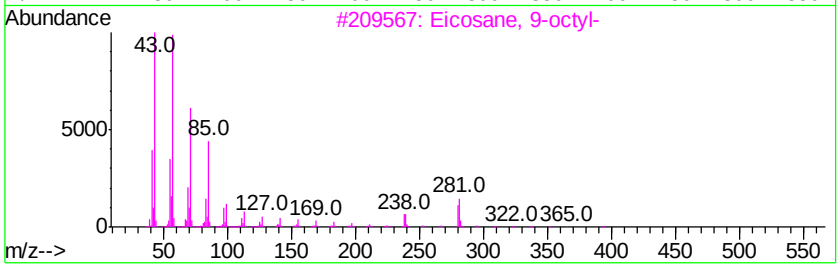
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.27	6.15 ng	91289	Perylene-d12	20.99

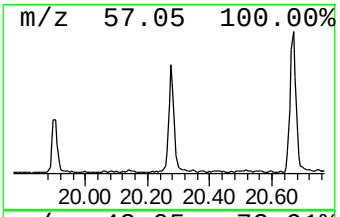
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	95
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
3	Eicosane, 9-octyl-	394	C28H58	013475-77-9	94
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	93
5	Hexacosane	366	C26H54	000630-01-3	91

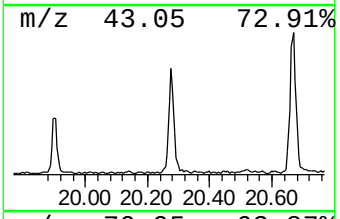


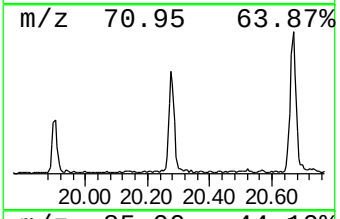


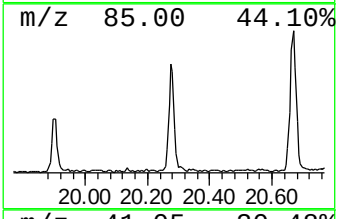


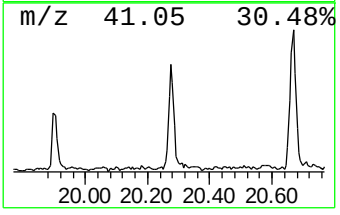












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

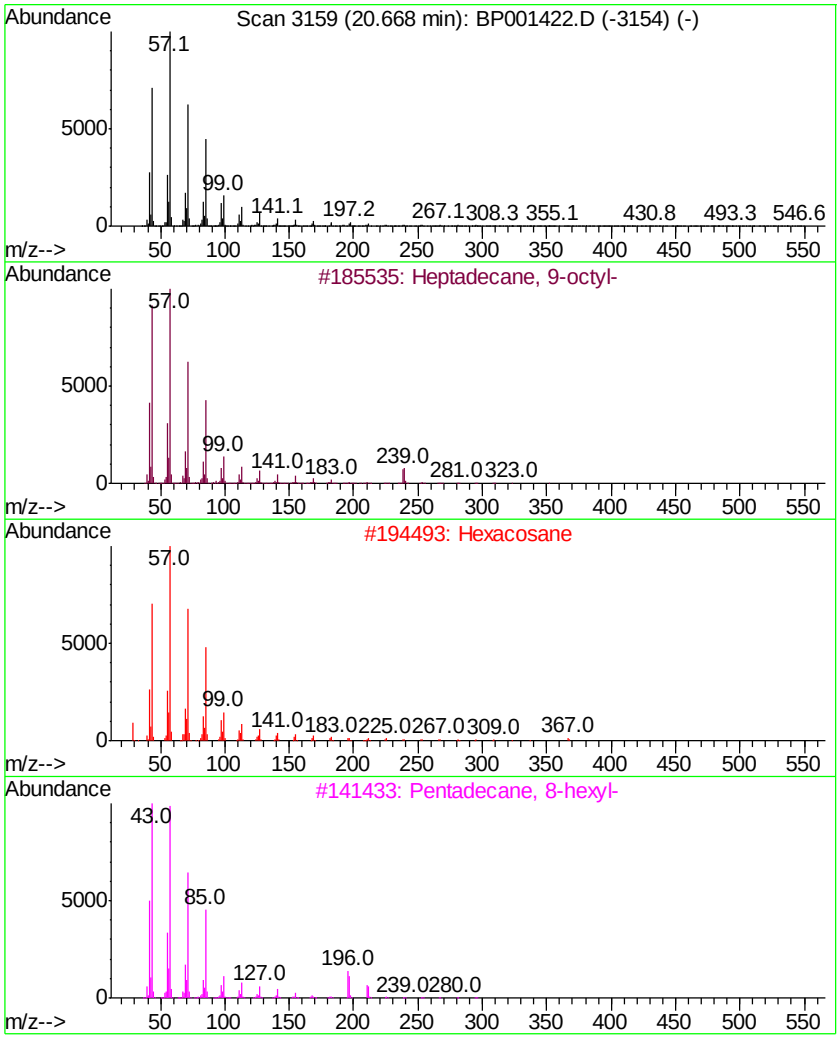
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

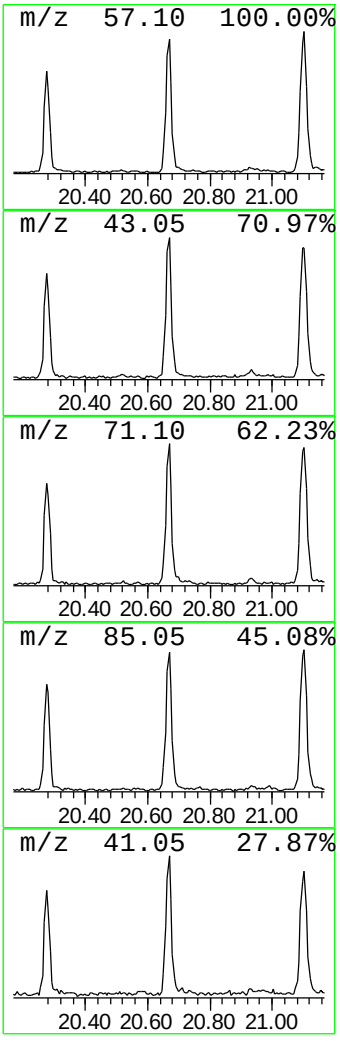
****

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.67	8.90 ng	132154	Perylene-d12	20.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2	Hexacosane	366	C26H54	000630-01-3	94
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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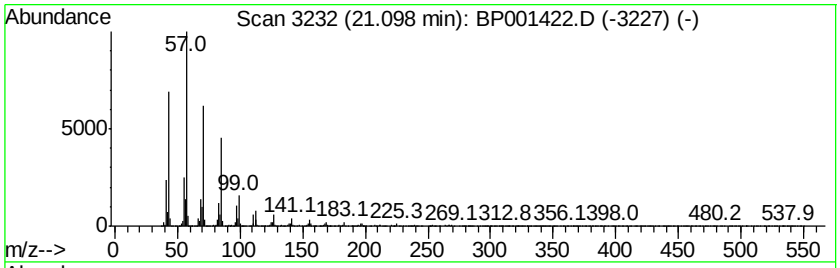
TIC Integration Parameters: LSCINT.P

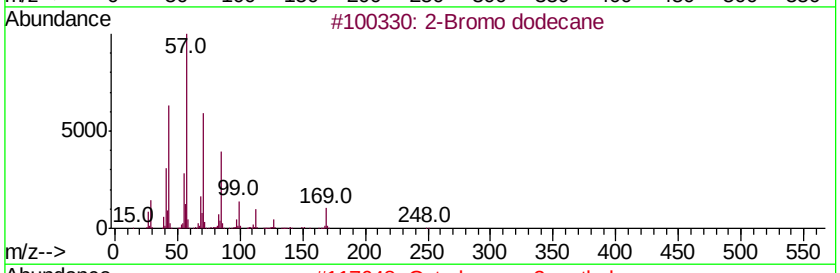
****

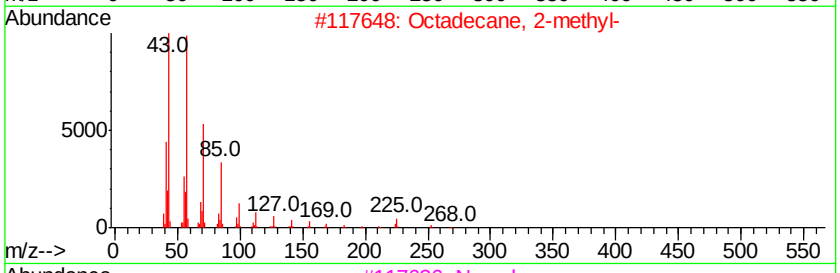
Peak Number 8 2-Bromo dodecane Concentration Rank 4

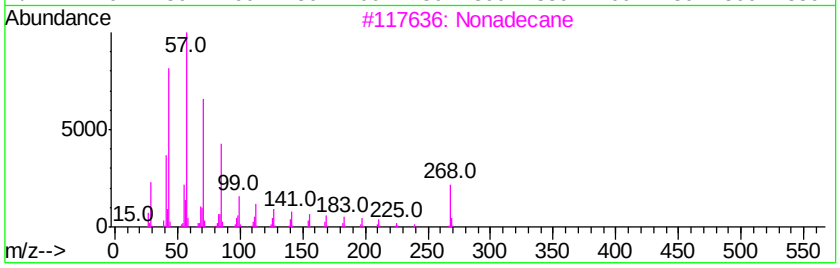
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.10	9.99 ng	148435	Perylene-d12	20.99

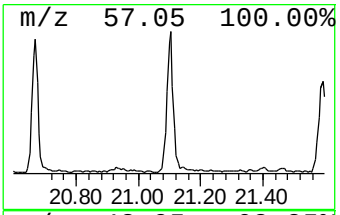
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	95
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
3	Nonadecane	268	C19H40	000629-92-5	93
4	Heptacosane	380	C27H56	000593-49-7	91
5	Pentacosane	352	C25H52	000629-99-2	91

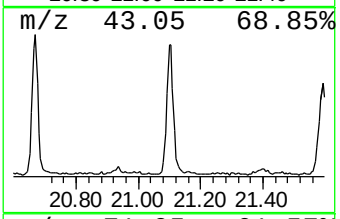


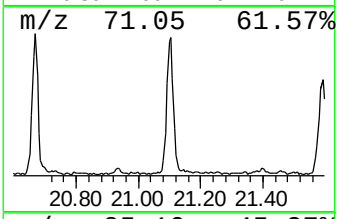


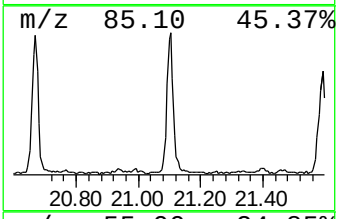


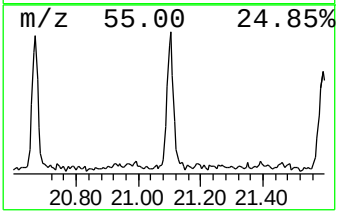












Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122619\
Data File : BP001422.D
Acq On : 26 Dec 2019 15:26
Operator : JU
Sample : PB125704BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB125704BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

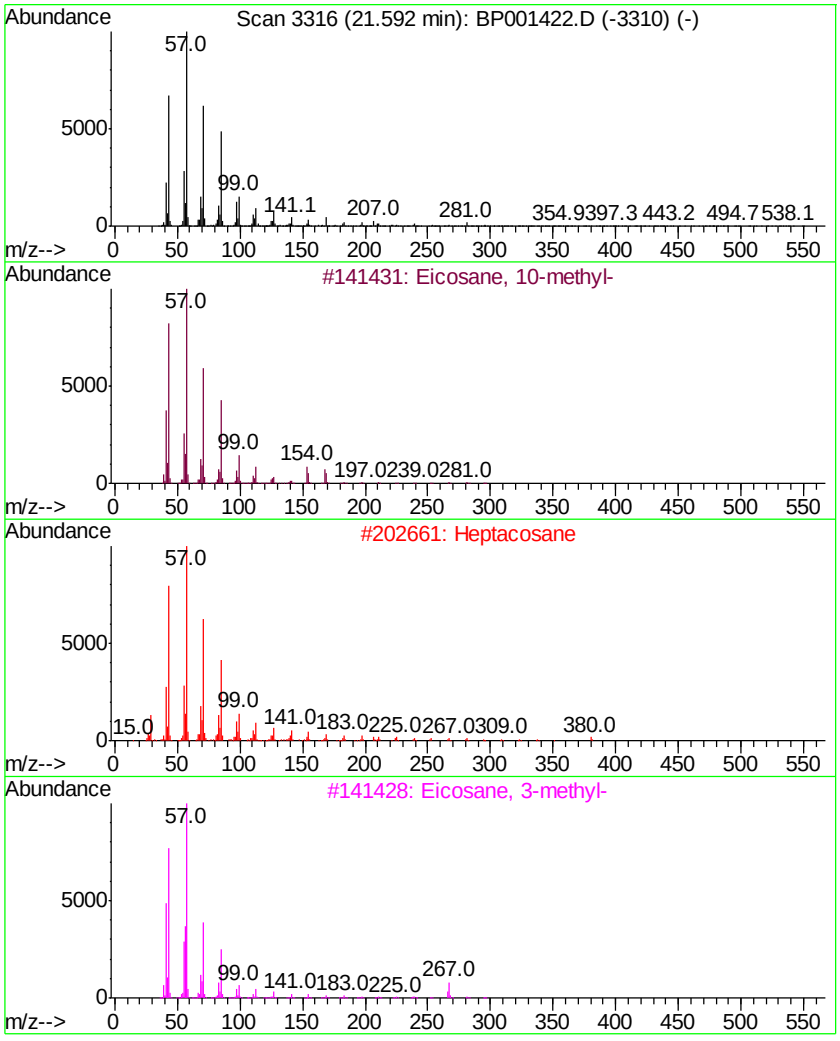
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

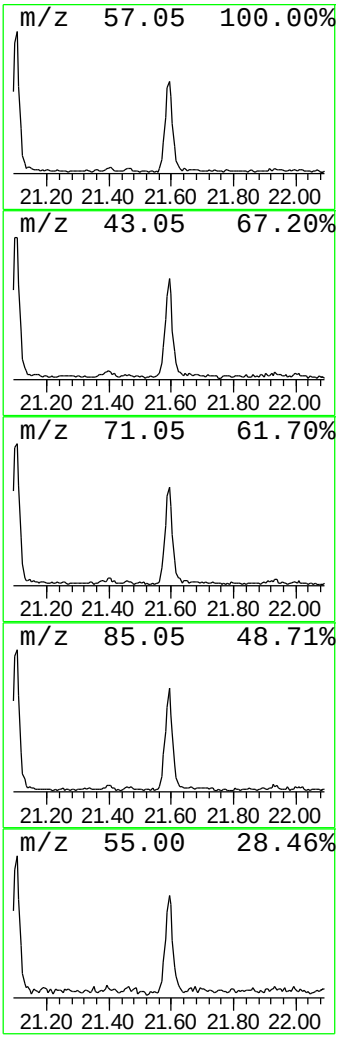
****

Peak Number 9 Eicosane, 10-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.59	7.59 ng	112767	Perylene-d12	20.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	Eicosane, 3-methyl-	296	C21H44	006418-46-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122619\
Data File : BP001422.D
Acq On : 26 Dec 2019 15:26
Operator : JU
Sample : PB125704BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB125704BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

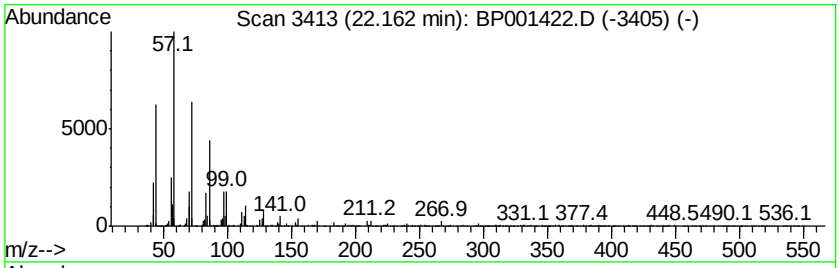
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

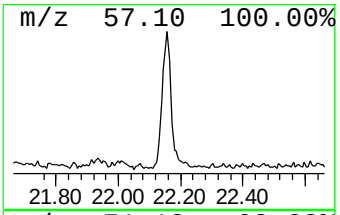
****

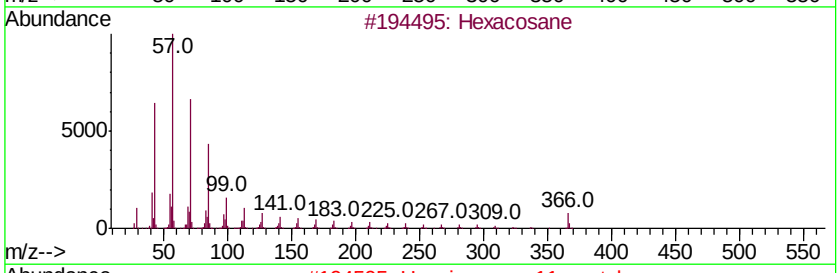
Peak Number 10 Hexacosane Concentration Rank 8

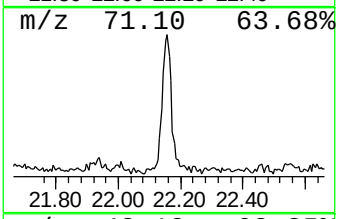
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.16	4.20 ng	62444	Perylene-d12	20.99

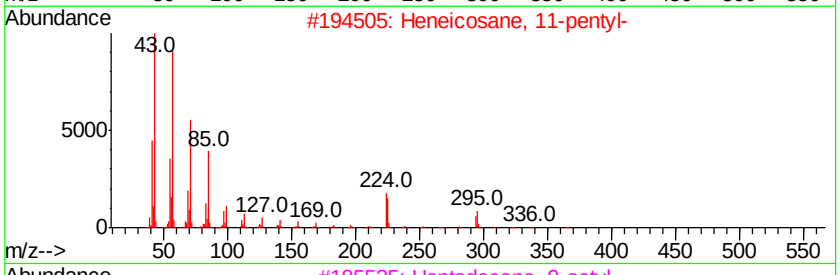
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90

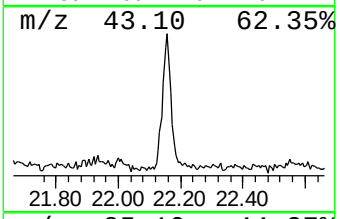


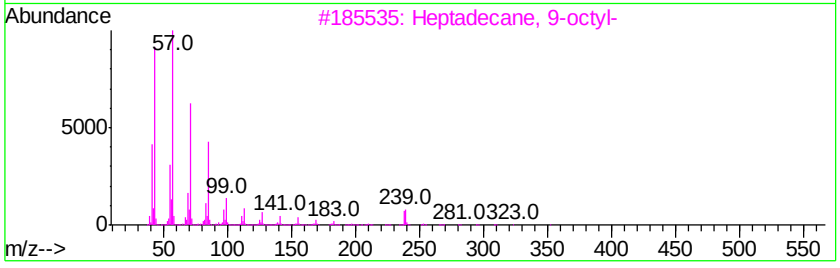


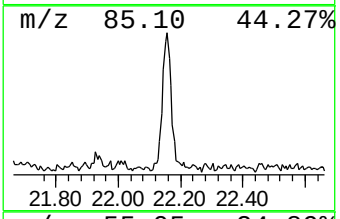


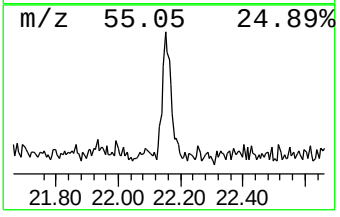












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP122619\
Data File : BP001422.D
Acq On : 26 Dec 2019 15:26
Operator : JU
Sample : PB125704BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PB125704BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.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-Pentanone, 4-hy...	5.59	11.1	ng	125830	1	8.28	227792	20.0
unknown7.93	7.93	109.0	ng	1241370	1	8.28	227792	20.0
Benzenamine, 2,4,...	15.72	2.7	ng	49499	4	15.58	366125	20.0
Docosane, 11-butyl-	19.90	2.8	ng	46222	5	19.22	332389	20.0
Tetracosane	20.27	6.2	ng	91289	6	20.99	297099	20.0
Heptadecane, 9-oc...	20.67	8.9	ng	132154	6	20.99	297099	20.0
2-Bromo dodecane	21.10	10.0	ng	148435	6	20.99	297099	20.0
Eicosane, 10-methyl-	21.59	7.6	ng	112767	6	20.99	297099	20.0
Hexacosane	22.16	4.2	ng	62444	6	20.99	297099	20.0